



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:45 pm BST

PDB ID : 3M32
Title : Structural Insight into Methyl-Coenzyme M Reductase Chemistry using Coenzyme B Analogues
Authors : Cedervall, P.E.; Dey, M.; Ragsdale, S.W.; Wilmot, C.M.
Deposited on : 2010-03-08
Resolution : 1.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

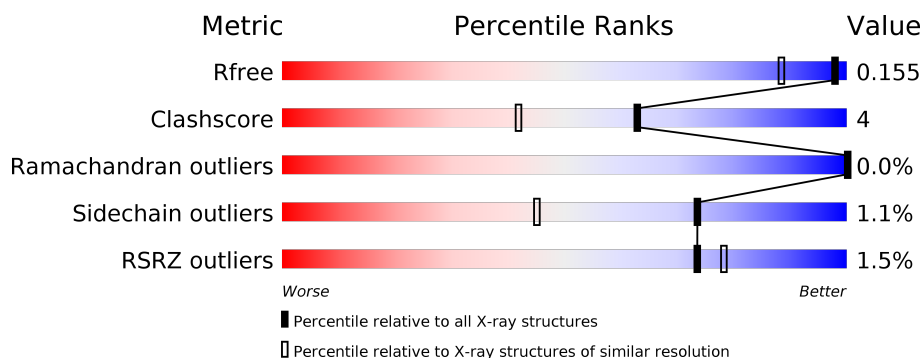
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	<div> <div style="width: 83%;"></div> <div style="width: 15%;"></div> <div style="width: 2%;"></div> </div> <div>83% 15% .</div>
1	D	549	<div> <div style="width: 83%;"></div> <div style="width: 15%;"></div> <div style="width: 2%;"></div> </div> <div>83% 15% .</div>
2	B	442	<div> <div style="width: 82%;"></div> <div style="width: 16%;"></div> <div style="width: 2%;"></div> </div> <div>82% 16% .</div>
2	E	442	<div> <div style="width: 84%;"></div> <div style="width: 15%;"></div> <div style="width: 1%;"></div> </div> <div>84% 15% .</div>
3	C	248	<div> <div style="width: 5%;"></div> <div style="width: 80%;"></div> <div style="width: 15%;"></div> <div style="width: 2%;"></div> </div> <div>5% 80% 18% .</div>
3	F	248	<div> <div style="width: 5%;"></div> <div style="width: 72%;"></div> <div style="width: 23%;"></div> <div style="width: 2%;"></div> </div> <div>5% 72% 25% ..</div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 22665 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Methyl-coenzyme M reductase I subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	28	0
			4431	2801	735	874	21			
1	D	548	Total	C	N	O	S	0	22	0
			4380	2779	727	853	21			

- Molecule 2 is a protein called Methyl-coenzyme M reductase I subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	24	0
			3462	2211	560	668	23			
2	E	442	Total	C	N	O	S	0	25	0
			3471	2216	564	668	23			

- Molecule 3 is a protein called Methyl-coenzyme M reductase I subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	0	10	0
			2056	1276	360	407	13			
3	F	246	Total	C	N	O	S	0	20	0
			2113	1309	372	418	14			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

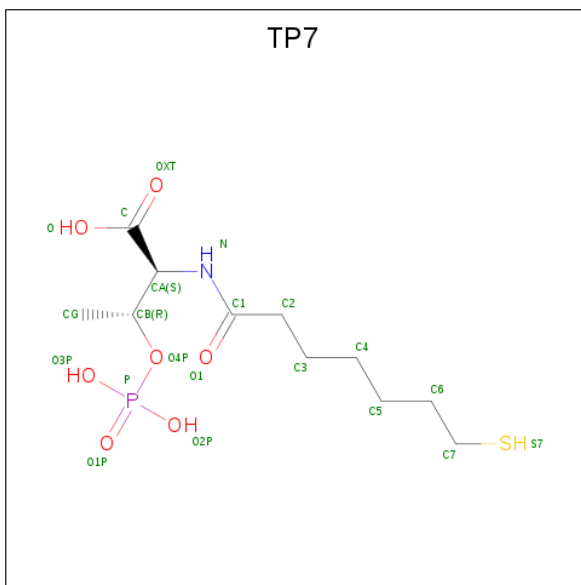
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		
4	E	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	1
			2	2		
4	C	1	Total	Mg	0	0
			1	1		

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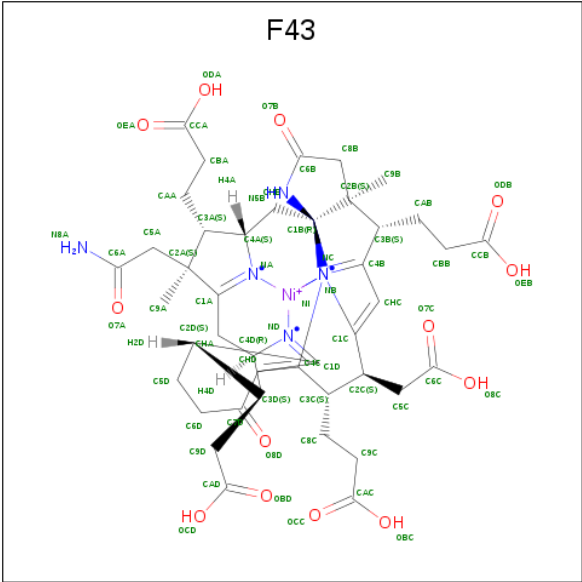
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	2
			2	2		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is Coenzyme B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



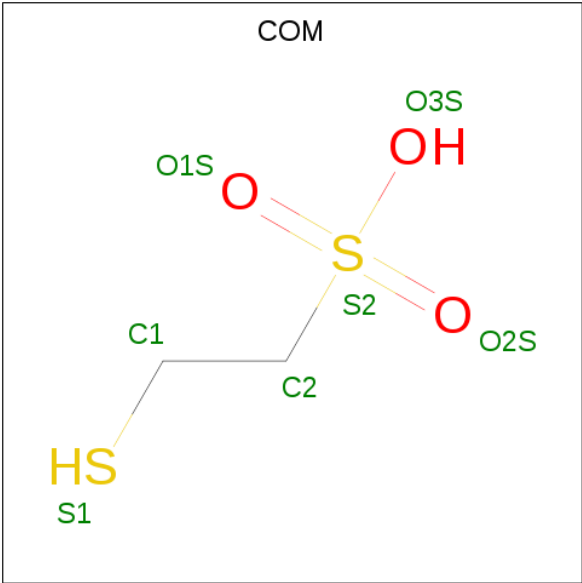
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	1
5	D	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	1

- Molecule 6 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



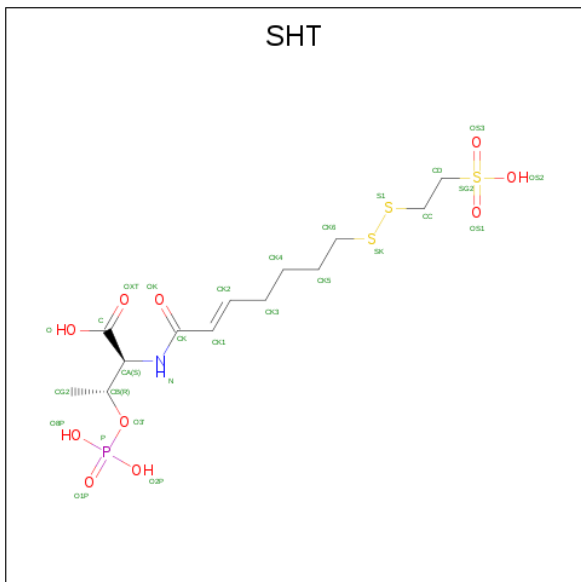
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
6	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 7 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: C₂H₆O₃S₂).



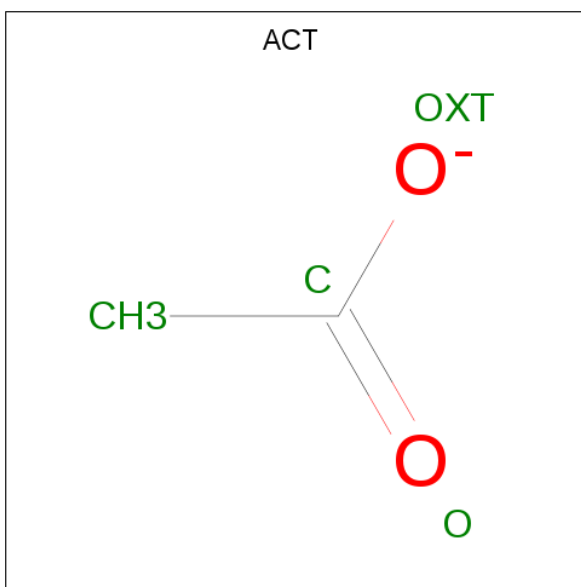
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	1
			7	2	3	2		
7	D	1	Total	C	O	S	0	1
			7	2	3	2		

- Molecule 8 is O-PHOSPHONO-N-{(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL}-L-THREONINE (three-letter code: SHT) (formula: $C_{13}H_{24}NO_{10}PS_3$).



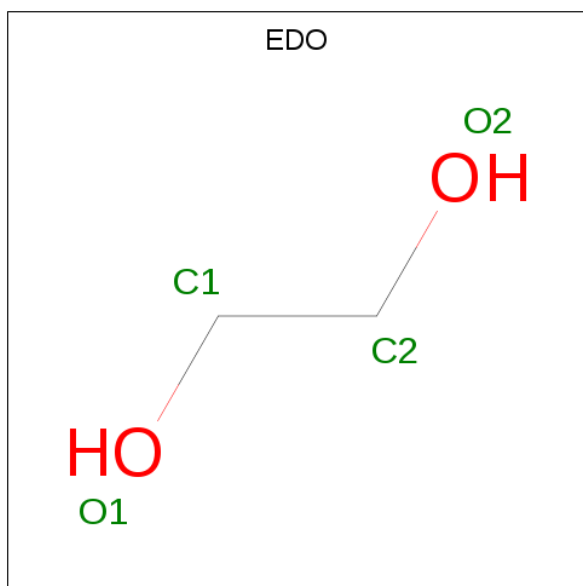
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			28	13	1	10	1	3		
8	D	1	Total	C	N	O	P	S	0	1
			28	13	1	10	1	3		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	1
			4	2	2		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Zn	0	0
			1	1		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			7	4	3		

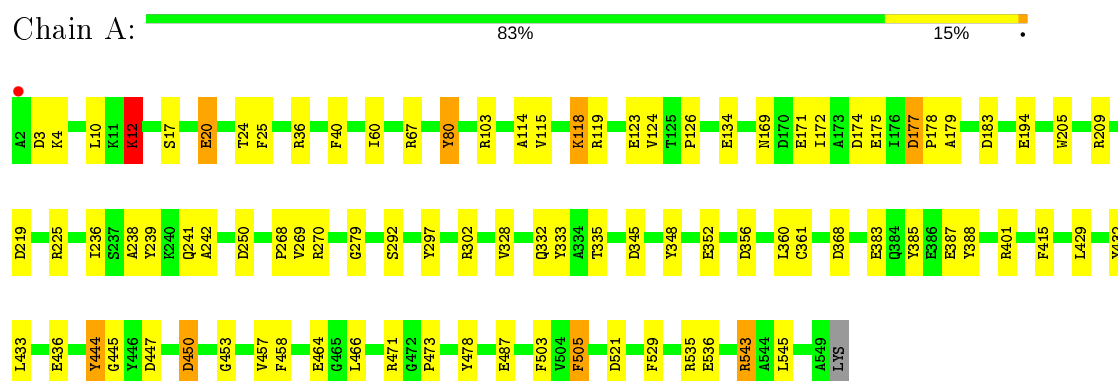
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	507	Total	O	0	28
			522	522		
13	B	462	Total	O	0	24
			477	477		
13	C	254	Total	O	0	12
			262	262		
13	D	529	Total	O	0	20
			539	539		
13	E	414	Total	O	0	16
			421	421		
13	F	250	Total	O	0	8
			254	254		

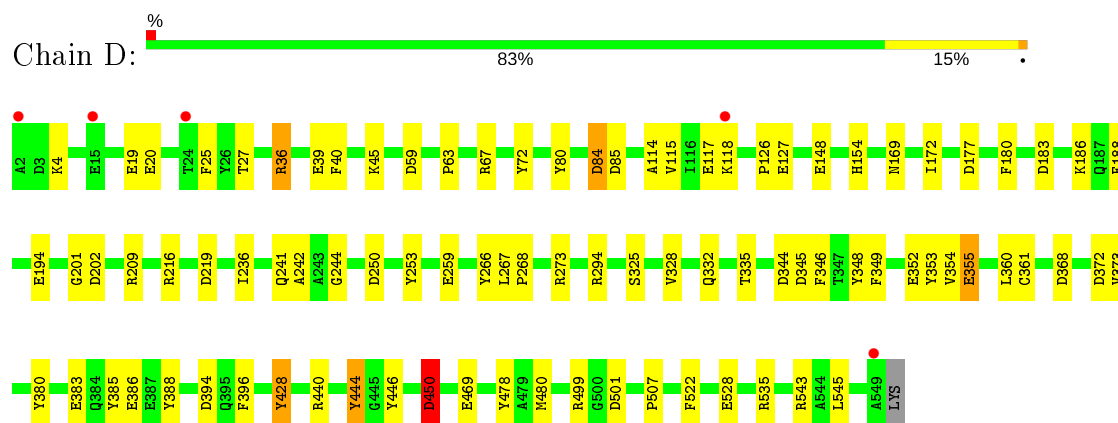
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

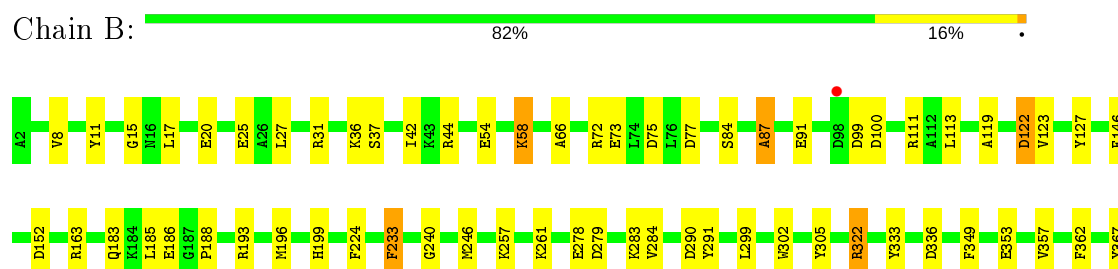
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



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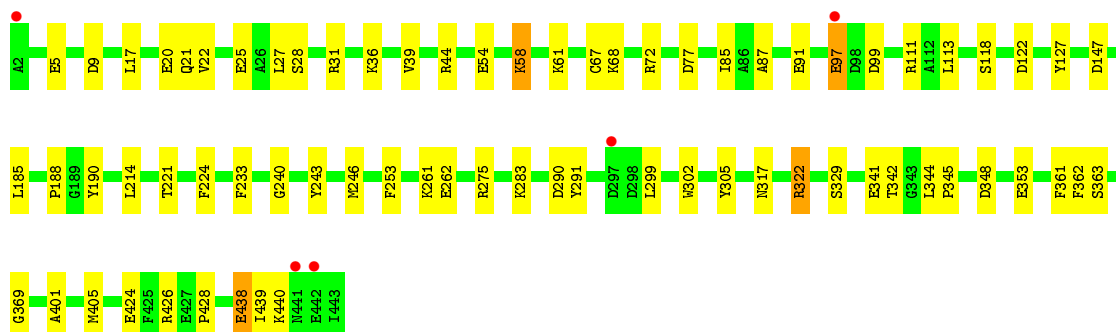
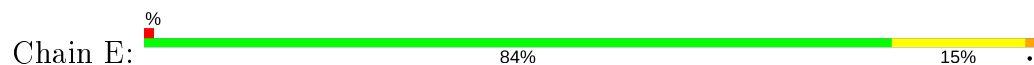


- Molecule 2: Methyl-coenzyme M reductase I subunit beta

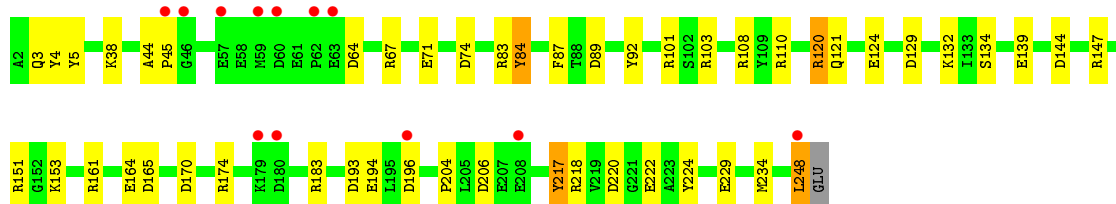
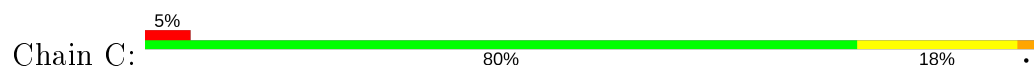




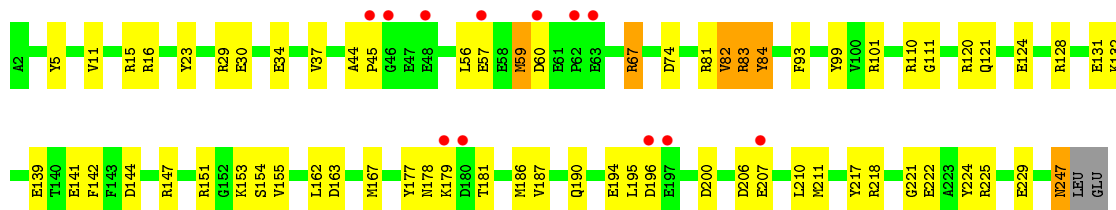
• Molecule 2: Methyl-coenzyme M reductase I subunit beta



• Molecule 3: Methyl-coenzyme M reductase I subunit gamma



• Molecule 3: Methyl-coenzyme M reductase I subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.02Å 118.26Å 122.39Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	20.28 – 1.35 19.89 – 1.35	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.28-1.35) 92.4 (19.89-1.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 1.35Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.140 , 0.157 0.139 , 0.155	Depositor DCC
R_{free} test set	23861 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k 0.006 for -h,-l,-k 0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22665	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PEG, SHT, SMC, ACT, MG, F43, MGN, TP7, AGM, EDO, GL3, COM, MHS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.58	28/4528 (0.6%)	1.45	44/6146 (0.7%)
1	D	1.62	29/4483 (0.6%)	1.52	55/6084 (0.9%)
2	B	1.58	27/3578 (0.8%)	1.49	37/4839 (0.8%)
2	E	1.65	28/3590 (0.8%)	1.41	25/4852 (0.5%)
3	C	1.80	20/2117 (0.9%)	1.63	29/2851 (1.0%)
3	F	1.84	31/2186 (1.4%)	1.68	40/2940 (1.4%)
All	All	1.65	163/20482 (0.8%)	1.51	230/27712 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	D	1	0
3	C	0	2
All	All	2	2

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	124	GLU	CG-CD	9.37	1.66	1.51
1	A	352	GLU	CD-OE2	9.14	1.35	1.25
3	F	139	GLU	CD-OE2	8.46	1.34	1.25
2	E	341	GLU	CD-OE2	8.21	1.34	1.25
1	D	386	GLU	CD-OE1	7.83	1.34	1.25
3	C	124	GLU	CD-OE2	-7.75	1.17	1.25
3	F	124	GLU	CG-CD	7.65	1.63	1.51
2	B	54	GLU	CD-OE1	-7.20	1.17	1.25
2	B	278	GLU	CD-OE2	7.18	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	194	GLU	CD-OE2	7.00	1.33	1.25
2	E	243	TYR	CD2-CE2	6.77	1.49	1.39
1	D	19	GLU	CD-OE1	6.74	1.33	1.25
1	A	450	ASP	CA-CB	-6.65	1.39	1.53
2	B	353	GLU	CD-OE1	-6.48	1.18	1.25
2	B	426	ARG	CZ-NH2	6.47	1.41	1.33
1	A	171	GLU	CD-OE1	6.46	1.32	1.25
1	D	259	GLU	CG-CD	6.45	1.61	1.51
2	E	58	LYS	CB-CG	-6.44	1.35	1.52
1	A	123	GLU	CD-OE2	6.42	1.32	1.25
1	A	297	TYR	CB-CG	-6.42	1.42	1.51
2	E	58	LYS	CD-CE	6.41	1.67	1.51
2	E	118	SER	CA-CB	6.40	1.62	1.52
3	F	225	ARG	CZ-NH1	-6.35	1.24	1.33
3	F	218	ARG	CZ-NH1	6.30	1.41	1.33
1	D	355[A]	GLU	CB-CG	-6.29	1.40	1.52
1	D	355[B]	GLU	CB-CG	-6.29	1.40	1.52
2	E	341	GLU	CD-OE1	-6.22	1.18	1.25
3	F	30	GLU	CD-OE2	6.20	1.32	1.25
1	A	238	ALA	C-O	6.18	1.35	1.23
2	E	85	ILE	N-CA	6.17	1.58	1.46
3	C	139	GLU	CD-OE2	6.15	1.32	1.25
1	D	126	PRO	CA-C	-6.12	1.40	1.52
2	B	367	TYR	CG-CD1	6.10	1.47	1.39
3	F	155	VAL	CB-CG2	6.09	1.65	1.52
1	A	123	GLU	CG-CD	6.08	1.61	1.51
2	E	22	VAL	CB-CG2	6.06	1.65	1.52
2	B	278	GLU	CD-OE1	6.05	1.32	1.25
3	C	134	SER	CB-OG	5.96	1.50	1.42
2	E	353	GLU	CG-CD	5.93	1.60	1.51
2	B	322	ARG	CZ-NH1	5.92	1.40	1.33
2	B	8	VAL	CA-CB	5.92	1.67	1.54
3	F	229	GLU	CD-OE2	5.92	1.32	1.25
2	E	253	PHE	CD1-CE1	5.91	1.51	1.39
3	F	221	GLY	C-O	5.86	1.33	1.23
1	A	236	ILE	C-O	5.85	1.34	1.23
1	D	383	GLU	CB-CG	-5.85	1.41	1.52
3	C	3	GLN	CB-CG	-5.82	1.36	1.52
2	E	21	GLN	CG-CD	5.81	1.64	1.51
2	E	233[A]	PHE	CD1-CE1	5.79	1.50	1.39
2	E	233[B]	PHE	CD1-CE1	5.79	1.50	1.39
1	A	444	TYR	CE2-CZ	-5.78	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	TYR	CG-CD1	5.76	1.46	1.39
1	A	464	GLU	CD-OE2	-5.76	1.19	1.25
3	C	229	GLU	CD-OE1	-5.76	1.19	1.25
1	D	450	ASP	CA-CB	-5.74	1.41	1.53
3	F	139	GLU	CD-OE1	-5.74	1.19	1.25
2	E	25	GLU	CD-OE2	5.73	1.31	1.25
2	B	440	LYS	CE-NZ	5.71	1.63	1.49
3	C	218	ARG	CZ-NH1	5.70	1.40	1.33
1	D	385	TYR	CD1-CE1	5.67	1.47	1.39
2	B	87	ALA	CA-CB	5.66	1.64	1.52
2	B	186	GLU	CD-OE1	-5.66	1.19	1.25
3	C	92	TYR	CE1-CZ	5.65	1.45	1.38
2	E	302	TRP	CG-CD1	5.65	1.44	1.36
1	A	134	GLU	CD-OE1	5.65	1.31	1.25
2	E	353	GLU	CD-OE1	-5.64	1.19	1.25
1	D	72	TYR	CG-CD2	5.63	1.46	1.39
3	C	4	TYR	CE2-CZ	-5.63	1.31	1.38
3	F	142	PHE	CE2-CZ	5.62	1.48	1.37
2	B	240	GLY	N-CA	5.62	1.54	1.46
1	A	269	VAL	CA-CB	5.61	1.66	1.54
2	B	291	TYR	CD1-CE1	5.60	1.47	1.39
3	F	141	GLU	CD-OE2	-5.58	1.19	1.25
3	F	210	LEU	N-CA	5.57	1.57	1.46
1	D	373	VAL	CB-CG2	5.56	1.64	1.52
3	F	84	TYR	CD2-CE2	-5.56	1.31	1.39
3	C	153	LYS	CE-NZ	5.56	1.62	1.49
1	D	469	GLU	CD-OE1	-5.54	1.19	1.25
3	F	224	TYR	CE1-CZ	5.54	1.45	1.38
1	D	63	PRO	CA-CB	5.54	1.64	1.53
2	E	329	SER	CB-OG	5.54	1.49	1.42
3	C	71	GLU	CB-CG	5.53	1.62	1.52
3	F	93	PHE	CD2-CE2	5.53	1.50	1.39
3	C	183	ARG	CZ-NH1	5.52	1.40	1.33
2	E	28	SER	CB-OG	5.50	1.49	1.42
1	D	446	TYR	CD1-CE1	5.47	1.47	1.39
1	D	543	ARG	CG-CD	-5.46	1.38	1.51
1	D	127	GLU	N-CA	-5.46	1.35	1.46
2	B	11	TYR	CE2-CZ	-5.46	1.31	1.38
1	D	39	GLU	CD-OE2	-5.46	1.19	1.25
3	C	87	PHE	CE2-CZ	5.45	1.47	1.37
3	C	120	ARG	CZ-NH1	5.44	1.40	1.33
1	A	388	TYR	CG-CD1	5.43	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	190	TYR	CG-CD1	5.43	1.46	1.39
1	A	25	PHE	CG-CD2	5.42	1.46	1.38
1	A	487	GLU	CD-OE2	5.42	1.31	1.25
3	C	204	PRO	N-CA	5.41	1.56	1.47
2	B	302	TRP	CG-CD1	5.41	1.44	1.36
1	A	36	ARG	CG-CD	5.39	1.65	1.51
1	A	503	PHE	CG-CD1	5.39	1.46	1.38
2	E	54	GLU	CD-OE1	-5.39	1.19	1.25
3	F	11	VAL	CB-CG1	5.39	1.64	1.52
1	A	119	ARG	CB-CG	-5.38	1.38	1.52
2	E	240	GLY	N-CA	5.38	1.54	1.46
3	F	23	TYR	CG-CD2	5.38	1.46	1.39
3	F	177	TYR	CZ-OH	5.37	1.47	1.37
1	A	444	TYR	CZ-OH	5.36	1.47	1.37
1	A	292	SER	CB-OG	5.36	1.49	1.42
3	C	38	LYS	CE-NZ	5.35	1.62	1.49
3	C	222	GLU	CD-OE2	5.34	1.31	1.25
2	B	433	VAL	CB-CG1	5.32	1.64	1.52
1	D	80	TYR	CD1-CE1	5.32	1.47	1.39
1	D	244	GLY	C-O	5.32	1.32	1.23
1	D	201	GLY	N-CA	5.32	1.54	1.46
2	B	25	GLU	CD-OE1	-5.32	1.19	1.25
3	C	164	GLU	CG-CD	5.32	1.59	1.51
1	D	20	GLU	CG-CD	5.30	1.59	1.51
1	A	387	GLU	CD-OE1	5.30	1.31	1.25
3	C	193	ASP	CB-CG	5.29	1.62	1.51
2	B	428	PRO	CA-CB	5.29	1.64	1.53
1	D	543	ARG	CB-CG	5.28	1.66	1.52
2	E	302	TRP	CD2-CE2	5.28	1.47	1.41
2	E	54	GLU	CB-CG	5.25	1.62	1.52
3	F	217	TYR	CG-CD1	5.25	1.46	1.39
2	B	73	GLU	CD-OE2	5.25	1.31	1.25
3	F	190	GLN	N-CA	5.25	1.56	1.46
3	C	174	ARG	NE-CZ	5.24	1.39	1.33
2	B	427	GLU	CG-CD	5.23	1.59	1.51
3	F	154	SER	CB-OG	5.22	1.49	1.42
1	A	536	GLU	CB-CG	5.21	1.62	1.52
2	E	87	ALA	CA-CB	5.21	1.63	1.52
3	F	99	TYR	CD1-CE1	5.20	1.47	1.39
3	F	84	TYR	CG-CD1	5.19	1.46	1.39
1	D	148	GLU	CD-OE2	5.19	1.31	1.25
2	E	5	GLU	CB-CG	5.19	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	TRP	CG-CD1	5.17	1.44	1.36
1	D	428	TYR	CG-CD1	5.16	1.45	1.39
1	A	297	TYR	CG-CD2	5.15	1.45	1.39
1	A	80	TYR	CD1-CE1	5.15	1.47	1.39
1	A	385	TYR	CE2-CZ	-5.13	1.31	1.38
1	D	354	VAL	CA-CB	5.13	1.65	1.54
1	D	352	GLU	CG-CD	5.12	1.59	1.51
3	F	82	VAL	CB-CG1	5.12	1.63	1.52
2	B	84	SER	CB-OG	-5.11	1.35	1.42
1	D	528	GLU	CD-OE1	5.11	1.31	1.25
2	B	58	LYS	CB-CG	-5.10	1.38	1.52
2	B	284	VAL	C-O	5.09	1.33	1.23
2	E	401	ALA	C-O	5.09	1.33	1.23
2	E	97	GLU	CD-OE1	5.09	1.31	1.25
2	E	363	SER	CB-OG	5.08	1.48	1.42
3	F	229	GLU	CB-CG	5.08	1.61	1.52
2	B	417	GLU	CG-CD	-5.06	1.44	1.51
1	D	353	TYR	CE2-CZ	5.06	1.45	1.38
3	F	37	VAL	CB-CG2	-5.04	1.42	1.52
3	F	222	GLU	CB-CG	5.04	1.61	1.52
2	B	146	PHE	CE1-CZ	5.03	1.47	1.37
3	F	101	ARG	NE-CZ	5.03	1.39	1.33
1	A	124	VAL	CB-CG2	5.03	1.63	1.52
2	B	36	LYS	CE-NZ	5.03	1.61	1.49
1	D	380	TYR	CE2-CZ	5.02	1.45	1.38
2	B	417	GLU	CD-OE2	5.01	1.31	1.25
3	F	34	GLU	CG-CD	5.01	1.59	1.51
3	F	187	VAL	CB-CG1	5.01	1.63	1.52

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	147	ARG	NE-CZ-NH1	16.68	128.64	120.30
2	B	44	ARG	NE-CZ-NH1	15.62	128.11	120.30
3	F	147	ARG	NE-CZ-NH1	14.07	127.33	120.30
1	D	499	ARG	NE-CZ-NH2	-13.57	113.52	120.30
2	B	44	ARG	NE-CZ-NH2	-12.99	113.80	120.30
3	F	206	ASP	CB-CG-OD1	12.62	129.66	118.30
3	F	144	ASP	CB-CG-OD2	10.59	127.83	118.30
2	B	31	ARG	NE-CZ-NH1	10.02	125.31	120.30
2	E	44	ARG	NE-CZ-NH1	9.58	125.09	120.30
2	E	44	ARG	NE-CZ-NH2	-9.54	115.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	101	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	D	440	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	B	72	ARG	NE-CZ-NH2	-9.20	115.70	120.30
2	E	353	GLU	OE1-CD-OE2	9.15	134.28	123.30
1	A	103	ARG	NE-CZ-NH2	-8.87	115.87	120.30
3	F	225	ARG	NE-CZ-NH2	-8.79	115.91	120.30
2	B	31	ARG	NE-CZ-NH2	-8.74	115.93	120.30
2	B	336	ASP	CB-CG-OD2	-8.69	110.48	118.30
3	C	144	ASP	CB-CG-OD2	8.54	125.99	118.30
2	E	111	ARG	NE-CZ-NH1	8.39	124.50	120.30
3	F	144	ASP	CB-CG-OD1	-8.23	110.89	118.30
3	C	83	ARG	NE-CZ-NH2	-8.20	116.20	120.30
3	F	196	ASP	CB-CG-OD1	8.11	125.60	118.30
3	C	147	ARG	NE-CZ-NH2	-8.02	116.29	120.30
3	F	218	ARG	NE-CZ-NH2	7.86	124.23	120.30
3	C	124	GLU	OE1-CD-OE2	7.66	132.49	123.30
3	C	161	ARG	NE-CZ-NH1	7.65	124.12	120.30
2	B	423	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	A	543	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	D	40	PHE	CB-CG-CD2	-7.46	115.58	120.80
1	A	521	ASP	CB-CG-OD1	7.41	124.97	118.30
1	D	444	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	D	368	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	D	385	TYR	CD1-CE1-CZ	-7.32	113.21	119.80
1	D	216	ARG	NE-CZ-NH1	7.32	123.96	120.30
3	C	161	ARG	NE-CZ-NH2	-7.30	116.65	120.30
3	F	59	MET	CG-SD-CE	-7.18	88.71	100.20
1	D	522	PHE	CB-CG-CD1	-7.18	115.78	120.80
3	F	15	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	A	209	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	450	ASP	CB-CA-C	7.00	124.39	110.40
1	D	344	ASP	CB-CG-OD1	-6.92	112.07	118.30
2	E	275	ARG	NE-CZ-NH2	-6.92	116.84	120.30
3	F	177	TYR	O-C-N	6.92	133.76	122.70
1	D	440	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	B	77	ASP	CB-CG-OD2	-6.87	112.12	118.30
3	F	147	ARG	NE-CZ-NH2	-6.87	116.86	120.30
2	E	426	ARG	NE-CZ-NH1	6.85	123.73	120.30
3	C	84	TYR	CB-CG-CD2	-6.85	116.89	121.00
3	C	144	ASP	CB-CG-OD1	-6.84	112.15	118.30
3	F	5	TYR	CB-CG-CD1	-6.83	116.90	121.00
1	A	209	ARG	NE-CZ-NH1	6.75	123.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	386	GLU	OE1-CD-OE2	-6.64	115.33	123.30
1	A	368	ASP	CB-CG-OD2	-6.53	112.42	118.30
2	E	147	ASP	CB-CG-OD1	6.52	124.17	118.30
2	E	322[A]	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	E	322[B]	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	B	193	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	B	163	ARG	NE-CZ-NH2	-6.46	117.07	120.30
3	C	224	TYR	CB-CG-CD1	6.45	124.87	121.00
1	D	368	ASP	CB-CG-OD1	6.44	124.10	118.30
1	D	535	ARG	NE-CZ-NH1	-6.42	117.09	120.30
3	F	229	GLU	OE1-CD-OE2	-6.38	115.64	123.30
3	F	29	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	F	128	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	D	346	PHE	CB-CG-CD2	-6.32	116.38	120.80
2	B	426	ARG	NE-CZ-NH1	6.31	123.45	120.30
3	F	222	GLU	OE1-CD-OE2	-6.29	115.75	123.30
3	C	151	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	E	122	ASP	CB-CG-OD1	6.25	123.92	118.30
1	D	202	ASP	CB-CG-OD1	6.23	123.91	118.30
2	B	152	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	529	PHE	CB-CG-CD2	-6.19	116.47	120.80
1	A	415	PHE	CB-CG-CD2	-6.18	116.47	120.80
1	D	294	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	D	67	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	E	185	LEU	CB-CG-CD1	6.15	121.45	111.00
3	F	16	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	501	ASP	CB-CG-OD1	6.13	123.81	118.30
3	F	101	ARG	NE-CZ-NH2	-6.13	117.24	120.30
2	E	348	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	40	PHE	CB-CG-CD2	-6.05	116.56	120.80
1	D	499	ARG	NH1-CZ-NH2	6.04	126.05	119.40
1	D	59	ASP	CB-CG-OD1	6.00	123.70	118.30
3	F	163	ASP	CB-CG-OD1	6.00	123.70	118.30
1	D	84	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	385	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	D	346	PHE	CB-CG-CD1	5.96	124.97	120.80
3	C	108	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	E	31	ARG	NE-CZ-NH1	5.94	123.27	120.30
3	F	110	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	447	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	294	ARG	NE-CZ-NH1	-5.92	117.34	120.30
2	E	9	ASP	CB-CG-OD2	-5.91	112.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	388	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	A	225	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	270	ARG	NE-CZ-NH1	5.87	123.23	120.30
3	C	217	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	20	GLU	OE1-CD-OE2	5.85	130.32	123.30
3	C	165	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	D	209	ARG	NE-CZ-NH1	5.84	123.22	120.30
3	F	131	GLU	OE1-CD-OE2	5.82	130.29	123.30
2	B	127	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	D	450	ASP	CB-CA-C	5.80	121.99	110.40
3	C	174	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	E	72	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	D	372	ASP	CB-CG-OD2	5.79	123.51	118.30
2	B	336	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	401	ARG	NE-CZ-NH2	5.76	123.18	120.30
2	E	243	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	A	250	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	80	TYR	CD1-CE1-CZ	-5.73	114.64	119.80
1	D	388	TYR	CD1-CE1-CZ	-5.71	114.66	119.80
1	A	471	ARG	NE-CZ-NH2	-5.71	117.45	120.30
3	F	83	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	D	478	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	D	180	PHE	CA-C-N	5.68	129.70	117.20
2	E	77	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	458	PHE	CB-CG-CD2	-5.67	116.83	120.80
2	B	400	ASP	CB-CG-OD1	-5.66	113.21	118.30
3	C	196	ASP	CB-CG-OD1	5.66	123.39	118.30
3	F	74	ASP	CB-CG-OD2	-5.63	113.23	118.30
2	E	291	TYR	CD1-CE1-CZ	-5.62	114.75	119.80
1	D	478	TYR	CB-CG-CD1	5.59	124.36	121.00
1	D	444	TYR	CB-CG-CD1	5.59	124.35	121.00
3	F	120	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	219	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	345	ASP	CB-CG-OD1	-5.57	113.28	118.30
2	B	152	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	119	ARG	NE-CZ-NH2	-5.55	117.52	120.30
3	F	224	TYR	CZ-CE2-CD2	5.55	124.79	119.80
3	C	120	ARG	NE-CZ-NH1	5.55	123.07	120.30
3	C	103	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	67	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	505	PHE	CB-CG-CD2	-5.53	116.93	120.80
3	F	167	MET	O-C-N	5.51	131.52	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253	TYR	CZ-CE2-CD2	-5.51	114.84	119.80
2	E	290	ASP	CB-CG-OD1	-5.50	113.35	118.30
2	B	305	TYR	CG-CD2-CE2	-5.50	116.90	121.30
2	E	361	PHE	CB-CG-CD2	-5.49	116.96	120.80
3	C	87	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	D	396	PHE	CZ-CE2-CD2	-5.49	113.52	120.10
3	C	129	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	238	ALA	CA-C-N	5.43	129.15	117.20
2	B	185	LEU	CB-CG-CD1	5.42	120.21	111.00
1	D	428	TYR	CB-CG-CD2	5.41	124.25	121.00
1	A	436	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	450	ASP	N-CA-CB	5.40	120.33	110.60
1	D	148	GLU	OE1-CD-OE2	-5.40	116.82	123.30
3	C	89	ASP	CB-CG-OD1	5.39	123.16	118.30
1	D	528	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	D	450	ASP	N-CA-CB	5.38	120.29	110.60
2	E	224	PHE	CB-CG-CD2	-5.38	117.03	120.80
3	F	16	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	B	99	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	10	LEU	O-C-N	5.37	131.29	122.70
3	C	217	TYR	CB-CG-CD2	5.36	124.21	121.00
2	B	75	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	478	TYR	CZ-CE2-CD2	-5.35	114.98	119.80
1	A	183	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	219	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	250	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	A	67	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	302	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	E	99	ASP	CB-CG-OD1	5.32	123.08	118.30
3	C	220	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	4	LYS	CA-CB-CG	5.31	125.08	113.40
3	F	162	LEU	CB-CG-CD2	5.30	120.02	111.00
3	F	110	ARG	CD-NE-CZ	5.30	131.02	123.60
3	F	81	ARG	NE-CZ-NH2	5.30	122.95	120.30
3	F	217	TYR	CB-CG-CD2	5.30	124.18	121.00
1	D	428	TYR	CB-CG-CD1	-5.29	117.83	121.00
2	B	333	TYR	CG-CD2-CE2	-5.29	117.07	121.30
2	B	291	TYR	CD1-CE1-CZ	-5.27	115.06	119.80
2	B	279	ASP	CB-CG-OD1	5.26	123.04	118.30
3	F	151	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	B	100	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	D	444	TYR	CD1-CE1-CZ	-5.24	115.09	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	478	TYR	CD1-CE1-CZ	-5.24	115.09	119.80
1	D	177	ASP	CB-CG-OD1	5.23	123.00	118.30
3	C	170	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	225	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	B	429	LEU	CB-CG-CD2	-5.20	102.16	111.00
3	C	110	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	12[A]	LYS	CD-CE-NZ	5.20	123.65	111.70
1	A	12[B]	LYS	CD-CE-NZ	5.20	123.65	111.70
2	B	224	PHE	CB-CG-CD2	-5.20	117.16	120.80
2	B	305	TYR	CD1-CE1-CZ	-5.19	115.13	119.80
1	A	333	TYR	CZ-CE2-CD2	-5.17	115.14	119.80
3	F	29	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	177[A]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	177[B]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	353	TYR	CZ-CE2-CD2	-5.16	115.15	119.80
3	F	151	ARG	CG-CD-NE	-5.16	100.96	111.80
1	A	348	TYR	CB-CG-CD2	-5.16	117.90	121.00
3	F	56	LEU	CB-CG-CD1	-5.15	102.24	111.00
2	E	58	LYS	CD-CE-NZ	5.15	123.54	111.70
1	D	349	PHE	O-C-N	-5.13	114.48	123.20
1	A	3	ASP	CB-CG-OD2	-5.13	113.69	118.30
3	F	141	GLU	CG-CD-OE1	-5.12	108.06	118.30
2	B	111	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	466	LEU	CB-CG-CD2	5.12	119.70	111.00
2	B	423	ASP	CB-CG-OD1	5.11	122.89	118.30
3	C	206	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	394	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	233[A]	PHE	CD1-CE1-CZ	-5.09	113.99	120.10
2	B	233[B]	PHE	CD1-CE1-CZ	-5.09	113.99	120.10
2	B	290	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	D	188	PHE	CB-CG-CD2	-5.09	117.24	120.80
3	F	195	LEU	CB-CG-CD1	-5.08	102.36	111.00
2	B	15	GLY	O-C-N	5.08	130.84	122.70
3	F	141	GLU	OE1-CD-OE2	5.08	129.40	123.30
2	E	127	TYR	CZ-CE2-CD2	-5.08	115.23	119.80
1	A	356	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	A	535	ARG	NE-CZ-NH1	-5.07	117.77	120.30
2	B	291	TYR	CB-CG-CD1	-5.07	117.96	121.00
3	C	5	TYR	CZ-CE2-CD2	-5.06	115.24	119.80
1	D	183	ASP	CB-CG-OD1	5.06	122.85	118.30
2	B	353	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	D	266	TYR	CD1-CE1-CZ	-5.05	115.25	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	74	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	345	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	A	238	ALA	CA-C-O	-5.02	109.56	120.10
2	E	305	TYR	CD1-CE1-CZ	-5.02	115.28	119.80
3	C	74	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	333	TYR	CG-CD2-CE2	5.01	125.31	121.30
3	F	30	GLU	CG-CD-OE1	5.01	128.31	118.30
2	B	122[A]	ASP	CB-CG-OD1	5.00	122.81	118.30
2	B	122[B]	ASP	CB-CG-OD1	5.00	122.81	118.30
1	D	183	ASP	CB-CG-OD2	-5.00	113.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	450	ASP	CA
1	D	450	ASP	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	120	ARG	Sidechain
3	C	217	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4431	0	4224	47	0
1	D	4380	0	4219	29	0
2	B	3462	0	3517	40	0
2	E	3471	0	3532	33	0
3	C	2056	0	2000	23	0
3	F	2113	0	2065	21	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	21	0	19	0	0
5	D	21	0	19	0	0
6	A	62	0	43	2	0
6	D	62	0	43	1	0
7	A	7	0	4	0	0
7	D	7	0	5	1	0
8	A	28	0	21	0	0
8	D	28	0	21	1	0
9	A	4	0	3	0	0
10	A	4	0	6	0	0
10	B	4	0	6	0	0
10	D	4	0	6	1	0
10	F	8	0	12	0	0
11	A	1	0	0	0	0
12	C	7	0	10	0	0
13	A	522	0	0	12	0
13	B	477	0	0	14	0
13	C	262	0	0	4	0
13	D	539	0	0	8	0
13	E	421	0	0	11	0
13	F	254	0	0	10	0
All	All	22665	0	19775	172	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:207[B]:GLU:HG3	13:F:3759:HOH:O	1.39	1.23
2:E:91[B]:GLU:HG2	13:E:3974:HOH:O	1.64	0.97
1:D:545[A]:LEU:HD12	13:D:2591:HOH:O	1.66	0.93
1:A:433:LEU:HD23	3:C:234[B]:MET:SD	2.08	0.93
1:A:433:LEU:CD2	3:C:234[B]:MET:SD	2.60	0.88
1:A:429:LEU:HD12	3:C:234[B]:MET:HE3	1.55	0.88
1:D:36[A]:ARG:HD3	1:D:85:ASP:OD1	1.76	0.86
2:E:438[A]:GLU:OE1	2:E:439:ILE:HG23	1.77	0.83
2:B:196[B]:MET:CE	13:B:3731:HOH:O	2.25	0.83
1:D:545[A]:LEU:CD1	13:D:2591:HOH:O	2.23	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67[B]:ARG:HG3	3:C:67[B]:ARG:HH11	1.44	0.81
3:C:67[B]:ARG:CG	3:C:67[B]:ARG:HH11	1.95	0.80
3:F:67[A]:ARG:HH11	3:F:67[A]:ARG:HG2	1.48	0.79
13:A:3768:HOH:O	1:D:545[A]:LEU:HD11	1.82	0.79
1:A:24[A]:THR:HG23	13:A:3803:HOH:O	1.84	0.77
2:B:196[B]:MET:CE	13:B:574:HOH:O	2.31	0.77
2:E:27:LEU:HD22	2:E:246[B]:MET:CE	2.16	0.75
1:A:429:LEU:HD12	3:C:234[B]:MET:CE	2.17	0.75
1:A:24[A]:THR:CG2	13:A:3803:HOH:O	2.35	0.73
2:E:261[A]:LYS:HG2	13:F:3664:HOH:O	1.88	0.73
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.70	0.73
2:B:196[B]:MET:HE3	13:B:574:HOH:O	1.88	0.72
2:B:27:LEU:HD22	2:B:246[B]:MET:CE	2.21	0.70
1:A:178[A]:PRO:HD3	13:A:1631:HOH:O	1.94	0.67
2:E:17:LEU:HD21	2:E:20[A]:GLU:HG3	1.77	0.67
2:B:299:LEU:HD23	2:B:349[A]:PHE:CE1	2.30	0.65
2:B:196[B]:MET:SD	13:B:3731:HOH:O	2.54	0.64
1:D:194[B]:GLU:HG2	13:D:3701:HOH:O	1.97	0.64
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	2.28	0.64
2:E:322[A]:ARG:CZ	3:F:67[A]:ARG:HD2	2.27	0.63
13:B:2205:HOH:O	2:E:188:PRO:HD3	1.98	0.63
1:D:268:PRO:HB3	13:E:1668:HOH:O	1.99	0.62
2:B:27:LEU:HD22	2:B:246[B]:MET:HE1	1.80	0.62
3:C:67[B]:ARG:NH1	3:C:67[B]:ARG:HB2	2.15	0.61
2:E:322[A]:ARG:NH1	3:F:67[A]:ARG:HD2	2.15	0.61
2:E:61[B]:LYS:CE	13:E:2444:HOH:O	2.49	0.61
1:A:429:LEU:CD1	3:C:234[B]:MET:CE	2.79	0.60
2:E:342:THR:OG1	2:E:344[B]:LEU:HB2	2.02	0.60
2:E:261[B]:LYS:O	2:E:261[B]:LYS:HD2	2.01	0.60
2:E:261[B]:LYS:HG3	2:E:262:GLU:HG3	1.82	0.60
1:A:241[B]:GLN:HA	13:F:4106:HOH:O	2.01	0.59
1:A:241[A]:GLN:HA	13:F:4106:HOH:O	2.02	0.59
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.43	0.59
1:A:114:ALA:O	1:A:118:LYS:HD3	2.02	0.59
2:B:196[B]:MET:HE1	13:B:3731:HOH:O	1.92	0.58
1:A:432:TYR:HB2	3:C:234[B]:MET:HE3	1.85	0.58
1:A:60:ILE:HD12	13:D:3878:HOH:O	2.04	0.58
1:A:169[A]:ASN:ND2	1:A:172:ILE:HD12	2.18	0.57
2:E:27:LEU:CD2	2:E:246[B]:MET:CE	2.82	0.57
3:C:67[B]:ARG:NH1	3:C:67[B]:ARG:CB	2.68	0.57
3:F:83:ARG:NH2	13:F:4106:HOH:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ALA:O	1:D:118:LYS:HD3	2.06	0.56
2:B:261[A]:LYS:HG3	13:B:4130:HOH:O	2.06	0.56
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:CB	2.18	0.56
3:F:57:GLU:HG2	13:F:939:HOH:O	2.06	0.56
1:A:241[B]:GLN:HB3	1:A:242:ALA:O	2.06	0.56
1:D:169[A]:ASN:CG	1:D:172:ILE:HG12	2.25	0.56
3:F:132[A]:LYS:HD2	13:F:1990:HOH:O	2.05	0.56
2:B:257:LYS:NZ	13:B:3430:HOH:O	2.38	0.55
1:D:360:LEU:O	1:D:361[A]:CYS:HB2	2.07	0.55
2:E:299:LEU:HD22	13:E:2973:HOH:O	2.07	0.55
1:A:360:LEU:O	1:A:361[B]:CYS:HB2	2.06	0.54
2:B:27:LEU:CD2	2:B:246[B]:MET:HE1	2.38	0.54
3:F:44:ALA:HB1	3:F:45:PRO:HD2	1.90	0.54
2:B:322:ARG:NH1	3:C:67[A]:ARG:HD3	2.23	0.54
3:C:194[B]:GLU:HG3	13:C:1318:HOH:O	2.08	0.54
2:B:119:ALA:HA	2:B:122[B]:ASP:OD2	2.06	0.53
1:A:17[A]:SER:OG	1:A:20:GLU:HG3	2.09	0.53
1:A:545:LEU:HD11	13:D:1948[B]:HOH:O	2.08	0.53
1:D:169[A]:ASN:OD1	1:D:172:ILE:HG12	2.09	0.53
1:A:383[A]:GLU:HG3	13:A:2606:HOH:O	2.09	0.53
1:A:4[A]:LYS:NZ	13:A:2253:HOH:O	2.42	0.52
2:B:58:LYS:HE2	13:B:3633:HOH:O	2.09	0.52
2:B:299:LEU:HD23	2:B:349[A]:PHE:HE1	1.71	0.52
2:B:233[B]:PHE:CE1	3:C:248:LEU:HG	2.44	0.52
1:A:174[A]:ASP:HB2	13:A:1937:HOH:O	2.10	0.51
1:A:194[B]:GLU:HG2	13:A:2095:HOH:O	2.11	0.50
1:A:328:VAL:HB	6:D:552:F43:H9A1	1.92	0.50
1:A:433:LEU:HD21	3:C:234[B]:MET:SD	2.48	0.50
3:F:67[A]:ARG:HH11	3:F:67[A]:ARG:CG	2.20	0.50
1:A:24[B]:THR:HG23	13:A:677:HOH:O	2.11	0.50
1:A:268:PRO:HG3	13:A:4030:HOH:O	2.11	0.50
2:B:199:HIS:CE1	2:B:415[B]:ILE:HD12	2.47	0.49
2:E:344[A]:LEU:HB3	2:E:345:PRO:HD2	1.93	0.49
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.47	0.49
3:F:200[A]:ASP:HB2	13:F:1920:HOH:O	2.11	0.49
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.47	0.49
1:A:169[A]:ASN:ND2	1:A:172:ILE:CD1	2.76	0.49
2:E:424[B]:GLU:HG3	13:E:3642:HOH:O	2.12	0.49
1:A:126:PRO:HB2	1:A:175[A]:GLU:HG2	1.94	0.49
1:A:432:TYR:HB2	3:C:234[B]:MET:CE	2.43	0.49
3:F:178[B]:ASN:HB3	3:F:181[B]:THR:OG1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:GLU:HB2	1:D:118:LYS:HD2	1.95	0.48
2:B:188:PRO:HD3	13:E:1304:HOH:O	2.12	0.48
2:B:261[A]:LYS:HE3	13:B:4130:HOH:O	2.14	0.48
2:B:299:LEU:HD23	2:B:349[A]:PHE:CZ	2.48	0.48
1:D:236:ILE:HA	1:D:241[A]:GLN:HB2	1.96	0.47
3:F:67[A]:ARG:NH1	3:F:67[A]:ARG:HG2	2.25	0.47
1:D:154:HIS:CE1	1:D:545[A]:LEU:HD21	2.49	0.47
2:E:299:LEU:CD2	13:E:2973:HOH:O	2.62	0.47
2:B:246[A]:MET:CE	2:B:429:LEU:HD12	2.45	0.47
1:D:169[A]:ASN:CG	1:D:172:ILE:CG1	2.83	0.47
2:B:113[A]:LEU:HD13	2:B:418:VAL:HG13	1.97	0.46
2:E:61[B]:LYS:HE2	13:E:2444:HOH:O	2.14	0.46
3:F:153[A]:LYS:NZ	13:F:1186:HOH:O	2.27	0.46
1:A:332:GLN:HA	1:A:335:THR:OG1	2.15	0.46
2:E:317:ASN:O	3:F:111:GLY:HA2	2.16	0.46
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:HB2	1.75	0.46
1:D:332:GLN:HA	1:D:335:THR:OG1	2.16	0.46
1:D:480:MET:O	8:D:555[B]:SHT:HK61	2.16	0.46
3:C:64[B]:ASP:HB2	13:C:3620:HOH:O	2.15	0.45
2:E:39:VAL:HG21	2:E:221:THR:HG21	1.98	0.45
3:F:67[A]:ARG:NH1	3:F:67[A]:ARG:CG	2.80	0.45
2:B:196[B]:MET:CE	13:B:1152:HOH:O	2.64	0.45
2:B:37:SER:OG	2:B:424[B]:GLU:OE1	2.21	0.45
1:D:36[A]:ARG:HG2	1:D:84:ASP:HB2	1.98	0.45
1:A:115:VAL:HG22	2:E:405[A]:MET:HG3	1.99	0.45
1:A:12[A]:LYS:HE2	1:A:80:TYR:CZ	2.52	0.45
1:A:177[B]:ASP:C	1:A:179:ALA:N	2.69	0.44
3:C:44:ALA:HB1	3:C:45:PRO:HD2	1.98	0.44
1:A:178[A]:PRO:HD2	13:A:1652:HOH:O	2.18	0.44
3:C:132:LYS:HE3	13:C:4098:HOH:O	2.18	0.44
3:F:82:VAL:O	3:F:83:ARG:HD2	2.16	0.44
2:B:87:ALA:O	2:B:91[B]:GLU:HG3	2.17	0.44
1:D:545[A]:LEU:HD11	13:D:2591:HOH:O	2.07	0.44
2:E:113[B]:LEU:HD23	2:E:113[B]:LEU:C	2.39	0.43
1:A:169[A]:ASN:HD22	1:A:172:ILE:HD12	1.82	0.43
1:A:60:ILE:CD1	13:D:3878:HOH:O	2.65	0.43
2:B:299:LEU:HD21	13:C:1043:HOH:O	2.17	0.43
2:B:42[A]:ILE:HG13	2:B:425:PHE:CE1	2.54	0.43
6:A:1:F43:H9A1	1:D:328:VAL:HB	2.01	0.43
2:B:27:LEU:CD2	2:B:246[B]:MET:CE	2.92	0.43
3:C:67[B]:ARG:CG	3:C:67[B]:ARG:NH1	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LEU:HD12	1:D:273:ARG:HB2	2.01	0.42
1:A:429:LEU:CD1	3:C:234[B]:MET:HE1	2.48	0.42
1:A:12[A]:LYS:HE2	1:A:80:TYR:CE1	2.54	0.42
2:B:17:LEU:HD21	2:B:20[A]:GLU:HG3	2.01	0.42
2:B:424[A]:GLU:HG3	13:B:3930:HOH:O	2.19	0.42
2:E:61[B]:LYS:HE2	2:E:68[B]:LYS:HE3	2.01	0.42
3:F:207[B]:GLU:CG	13:F:3759:HOH:O	2.24	0.42
2:E:20[B]:GLU:HG2	13:E:768:HOH:O	2.19	0.42
2:E:61[B]:LYS:HE3	13:E:2370:HOH:O	2.20	0.42
1:A:505:PHE:CE1	2:E:67:CYS:HB3	2.54	0.42
2:B:246[B]:MET:HB3	2:B:246[B]:MET:HE3	1.66	0.42
1:A:279:GLY:HA2	1:A:473:PRO:HB2	2.01	0.42
1:D:241[A]:GLN:HB3	1:D:242:ALA:O	2.20	0.42
2:E:214:LEU:HB2	2:E:428:PRO:HG3	2.02	0.42
2:E:61[A]:LYS:HB3	2:E:61[A]:LYS:HE3	1.95	0.42
1:A:12[A]:LYS:HG2	1:A:80:TYR:CD2	2.55	0.42
1:D:45[A]:LYS:HE2	1:D:45[A]:LYS:HB3	1.78	0.42
1:D:348:TYR:CZ	10:D:556:EDO:H11	2.55	0.41
1:A:172:ILE:HD12	13:A:3660:HOH:O	2.20	0.41
1:A:126:PRO:CB	1:A:175[A]:GLU:HG2	2.51	0.41
2:B:123[B]:VAL:HG12	2:E:36:LYS:HA	2.01	0.41
1:D:25:PHE:O	1:D:27:THR:HG23	2.21	0.41
2:B:362:PHE:O	2:B:369:GLY:HA3	2.20	0.41
2:B:405[A]:MET:HG3	1:D:115:VAL:HG22	2.02	0.41
3:F:59:MET:O	3:F:60:ASP:C	2.57	0.41
2:B:119:ALA:O	2:B:122[B]:ASP:HB2	2.21	0.41
1:A:445:GL3:HA2	2:B:357:VAL:HG12	2.02	0.41
3:F:247:ASN:C	3:F:247:ASN:HD22	2.24	0.41
1:A:453:GLY:O	1:A:457:VAL:HG23	2.21	0.41
2:B:122[B]:ASP:HB2	13:B:1261:HOH:O	2.20	0.41
6:A:1:F43:C1C	7:D:554[A]:COM:H12	2.51	0.40
2:B:183:GLN:HG2	13:E:1668:HOH:O	2.19	0.40
1:D:355[B]:GLU:HG2	13:D:1824:HOH:O	2.21	0.40
1:D:428:TYR:HD1	1:D:450:ASP:HB3	1.86	0.40
2:B:261[A]:LYS:CE	13:B:4130:HOH:O	2.70	0.40
2:B:66:ALA:O	1:D:507:PRO:HD2	2.22	0.40
2:E:362:PHE:O	2:E:369:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	569/549 (104%)	555 (98%)	14 (2%)	0	100	100
1	D	563/549 (103%)	544 (97%)	18 (3%)	1 (0%)	47	21
2	B	465/442 (105%)	457 (98%)	8 (2%)	0	100	100
2	E	466/442 (105%)	457 (98%)	9 (2%)	0	100	100
3	C	255/248 (103%)	247 (97%)	8 (3%)	0	100	100
3	F	264/248 (106%)	258 (98%)	6 (2%)	0	100	100
All	All	2582/2478 (104%)	2518 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	325	SER

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	461/434 (106%)	455 (99%)	6 (1%)	69	37
1	D	455/434 (105%)	450 (99%)	5 (1%)	73	45
2	B	366/341 (107%)	365 (100%)	1 (0%)	92	83
2	E	367/341 (108%)	361 (98%)	6 (2%)	62	30
3	C	225/216 (104%)	223 (99%)	2 (1%)	78	53
3	F	233/216 (108%)	226 (97%)	7 (3%)	41	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2107/1982 (106%)	2080 (99%)	27 (1%)	73 37

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12[A]	LYS
1	A	12[B]	LYS
1	A	118	LYS
1	A	444	TYR
1	A	450	ASP
1	A	543	ARG
2	B	283	LYS
3	C	121	GLN
3	C	248	LEU
1	D	36[A]	ARG
1	D	36[B]	ARG
1	D	186	LYS
1	D	444	TYR
1	D	450	ASP
2	E	58	LYS
2	E	97	GLU
2	E	283	LYS
2	E	438[A]	GLU
2	E	438[B]	GLU
2	E	440	LYS
3	F	67[A]	ARG
3	F	67[B]	ARG
3	F	121	GLN
3	F	179[A]	LYS
3	F	179[B]	LYS
3	F	186	MET
3	F	247	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	121	GLN
3	F	121	GLN
3	F	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	MHS	A	257	1	7,11,12	1.63	2 (28%)	6,14,16	3.87	3 (50%)
1	AGM	A	271	1	10,11,12	0.81	0	6,13,15	1.97	1 (16%)
1	SMC	A	452	1	5,6,7	1.21	1 (20%)	2,6,8	2.28	1 (50%)
1	MGN	D	400	1	6,9,10	1.80	2 (33%)	5,12,14	0.79	0
1	GL3	A	445	1	2,3,4	2.45	1 (50%)	1,2,4	0.24	0
1	GL3	D	445	1	2,3,4	2.66	1 (50%)	1,2,4	0.26	0
1	MGN	A	400	1	6,9,10	1.23	1 (16%)	5,12,14	0.39	0
1	MHS	D	257	1	7,11,12	1.36	1 (14%)	6,14,16	3.84	2 (33%)
1	SMC	D	452	1	5,6,7	1.25	0	2,6,8	1.90	1 (50%)
1	AGM	D	271	1	10,11,12	0.96	0	6,13,15	1.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	AGM	A	271	1	-	3/10/11/13	-
1	SMC	A	452	1	-	1/3/5/7	-
1	MGN	D	400	1	-	0/7/9/12	-
1	GL3	A	445	1	-	1/1/1/2	-
1	GL3	D	445	1	-	0/1/1/2	-
1	MGN	A	400	1	-	0/7/9/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	SMC	D	452	1	-	1/3/5/7	-
1	AGM	D	271	1	-	1/10/11/13	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	GL3	C-S	-3.76	1.67	1.80
1	A	445	GL3	C-S	-3.46	1.68	1.80
1	A	257	MHS	CE1-NE2	3.17	1.41	1.34
1	D	400	MGN	CB1-CA	-3.00	1.51	1.55
1	D	257	MHS	CE1-NE2	2.79	1.41	1.34
1	A	400	MGN	CB1-CA	2.55	1.57	1.55
1	D	400	MGN	O-C	2.34	1.27	1.19
1	A	257	MHS	O-C	2.12	1.28	1.19
1	A	452	SMC	CB-CA	2.03	1.58	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MHS	NE2-CE1-ND1	-7.82	100.64	112.26
1	A	257	MHS	NE2-CE1-ND1	-7.82	100.65	112.26
1	D	257	MHS	CD2-NE2-CE1	4.22	112.36	105.78
1	A	257	MHS	CB-CA-C	-3.79	104.37	111.47
1	A	271	AGM	NH1-CZ-NE1	3.47	127.31	119.55
1	A	452	SMC	CA-CB-SG	-3.22	108.83	114.04
1	A	257	MHS	CD2-NE2-CE1	3.05	110.53	105.78
1	D	452	SMC	CA-CB-SG	-2.47	110.04	114.04

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	452	SMC	CA-CB-SG-CS
1	D	452	SMC	CA-CB-SG-CS
1	A	445	GL3	S-C-CA-N
1	A	271	AGM	CE2-CD-NE1-CZ
1	D	271	AGM	CE2-CD-NE1-CZ
1	A	271	AGM	CE2-CD-CG-CB
1	A	271	AGM	NE1-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	445	GL3	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	EDO	F	251	-	3,3,3	0.68	0	2,2,2	0.47	0
10	EDO	D	556	-	3,3,3	0.36	0	2,2,2	0.38	0
6	F43	A	1	1,8,7	46,71,71	2.99	11 (23%)	48,118,118	1.64	11 (22%)
10	EDO	F	1	-	3,3,3	0.58	0	2,2,2	0.53	0
10	EDO	A	557	-	3,3,3	0.59	0	2,2,2	0.33	0
10	EDO	B	445	-	3,3,3	0.75	0	2,2,2	0.29	0
8	SHT	D	555[B]	6	23,27,27	2.82	3 (13%)	25,36,36	2.09	5 (20%)
9	ACT	A	556[B]	4	1,3,3	1.15	0	0,3,3	0.00	-
7	COM	D	554[A]	6	6,6,6	1.51	1 (16%)	7,8,8	0.83	0
5	TP7	D	553[A]	-	16,20,20	1.03	1 (6%)	18,26,26	1.22	2 (11%)
5	TP7	A	553[A]	-	16,20,20	0.93	0	18,26,26	1.52	4 (22%)
7	COM	A	554[A]	6	6,6,6	1.52	1 (16%)	7,8,8	1.66	1 (14%)
12	PEG	C	1	-	6,6,6	0.55	0	5,5,5	1.14	1 (20%)
6	F43	D	552	1,8,7	46,71,71	3.32	15 (32%)	48,118,118	2.16	15 (31%)
8	SHT	A	555[B]	6	23,27,27	3.14	5 (21%)	25,36,36	2.07	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	F	251	-	-	1/1/1/1	-
10	EDO	D	556	-	-	1/1/1/1	-
6	F43	A	1	1,8,7	-	1/18/185/185	-
10	EDO	F	1	-	-	1/1/1/1	-
10	EDO	A	557	-	-	1/1/1/1	-
10	EDO	B	445	-	-	1/1/1/1	-
8	SHT	D	555[B]	6	-	4/27/31/31	-
7	COM	D	554[A]	6	-	0/4/4/4	-
5	TP7	D	553[A]	-	-	1/20/24/24	-
5	TP7	A	553[A]	-	-	2/20/24/24	-
7	COM	A	554[A]	6	-	0/4/4/4	-
12	PEG	C	1	-	-	0/4/4/4	-
6	F43	D	552	1,8,7	-	1/18/185/185	-
8	SHT	A	555[B]	6	-	5/27/31/31	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	555[B]	SHT	CD-SG2	-11.77	1.60	1.77
6	D	552	F43	NI-NB	11.71	2.14	1.89
6	D	552	F43	NI-NA	9.87	2.10	1.89
6	A	1	F43	NI-NB	9.64	2.10	1.89
6	A	1	F43	CHB-C1B	-9.55	1.46	1.53
8	D	555[B]	SHT	CD-SG2	-9.16	1.64	1.77
6	A	1	F43	NI-NA	8.77	2.08	1.89
8	D	555[B]	SHT	CK1-CK2	8.20	1.53	1.32
6	D	552	F43	NI-ND	8.10	2.07	1.89
8	A	555[B]	SHT	CK1-CK2	7.88	1.52	1.32
6	D	552	F43	CHD-C1D	7.60	1.53	1.43
6	A	1	F43	NI-ND	6.79	2.04	1.89
6	A	1	F43	CHA-C4D	4.49	1.57	1.53
6	D	552	F43	C3C-C4C	4.32	1.57	1.50
6	D	552	F43	C6D-C7D	-4.20	1.45	1.50
8	D	555[B]	SHT	OS3-SG2	4.07	1.57	1.45
6	A	1	F43	C3C-C4C	3.56	1.56	1.50
6	D	552	F43	O8D-C7D	3.40	1.30	1.23
6	D	552	F43	CHC-C1C	-3.13	1.29	1.36
6	D	552	F43	C1C-NC	3.12	1.44	1.37
7	A	554[A]	COM	C2-S2	-3.03	1.73	1.77
6	D	552	F43	C8C-C3C	2.85	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	552	F43	C3C-C2C	-2.82	1.47	1.54
6	D	552	F43	C9D-C3D	-2.82	1.50	1.54
6	A	1	F43	CHC-C4B	2.71	1.46	1.39
6	A	1	F43	C5D-C2D	2.68	1.58	1.53
6	A	1	F43	O8D-C7D	2.63	1.28	1.23
6	A	1	F43	C4A-NA	2.51	1.53	1.49
6	D	552	F43	CHB-C1B	2.51	1.55	1.53
6	A	1	F43	C5C-C2C	-2.44	1.50	1.54
6	D	552	F43	C5C-C2C	2.35	1.57	1.54
6	D	552	F43	C6B-N5B	-2.30	1.31	1.34
8	A	555[B]	SHT	CG2-CB	2.25	1.57	1.51
5	D	553[A]	TP7	C7-S7	2.16	1.88	1.80
7	D	554[A]	COM	C2-S2	-2.10	1.74	1.77
8	A	555[B]	SHT	P-O1P	2.06	1.57	1.50
8	A	555[B]	SHT	CC-CD	2.01	1.57	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	555[B]	SHT	CK3-CK2-CK1	-6.95	110.95	125.85
6	D	552	F43	C5D-C2D-C1D	6.17	118.75	110.45
6	D	552	F43	C2D-C1D-CHD	-5.62	114.66	121.85
8	A	555[B]	SHT	OS2-SG2-CD	4.93	113.74	105.77
8	A	555[B]	SHT	CK3-CK2-CK1	-4.84	115.46	125.85
8	A	555[B]	SHT	OS3-SG2-CD	4.80	112.69	106.92
6	A	1	F43	CAB-C3B-C2B	-4.60	109.36	119.09
6	D	552	F43	C1D-CHD-C4C	-4.28	113.14	125.31
6	D	552	F43	C6D-C7D-CHD	4.07	124.60	116.95
8	D	555[B]	SHT	OS2-SG2-CD	4.06	112.34	105.77
6	D	552	F43	C7D-CHD-C4C	3.75	129.52	121.61
7	A	554[A]	COM	O1S-S2-C2	-3.72	102.43	106.92
5	A	553[A]	TP7	CB-CA-N	3.72	119.68	111.38
6	D	552	F43	O7B-C6B-N5B	-3.53	120.54	125.13
6	D	552	F43	C2B-C3B-C4B	3.53	105.61	101.63
8	D	555[B]	SHT	OS2-SG2-OS3	3.39	119.56	111.27
6	A	1	F43	C4A-NA-C1A	-3.36	104.89	108.97
5	D	553[A]	TP7	CB-CA-N	3.33	118.81	111.38
6	D	552	F43	C4B-CHC-C1C	3.29	131.22	125.84
8	D	555[B]	SHT	OS1-SG2-OS3	-3.00	103.55	113.95
6	A	1	F43	C6D-C7D-CHD	2.91	122.43	116.95
6	D	552	F43	C2B-C1B-NB	2.85	106.10	101.84
5	A	553[A]	TP7	C2-C1-N	2.83	120.75	115.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1	F43	C3D-C4D-ND	2.83	106.74	102.34
6	D	552	F43	CAB-C3B-C2B	-2.78	113.20	119.09
6	A	1	F43	O8D-C7D-C6D	-2.76	116.34	120.86
6	D	552	F43	O8D-C7D-CHD	-2.72	118.10	122.75
6	A	1	F43	C9B-C2B-C3B	2.64	119.70	112.96
8	A	555[B]	SHT	OS2-SG2-OS1	-2.56	105.03	111.27
5	A	553[A]	TP7	O4P-P-O1P	-2.42	100.04	109.39
6	A	1	F43	C9B-C2B-C8B	-2.41	104.37	110.45
6	A	1	F43	C3B-C4B-CHC	-2.34	118.27	123.32
6	D	552	F43	C3D-C2D-C1D	-2.34	98.73	102.69
8	A	555[B]	SHT	CK1-CK-N	2.32	119.02	114.56
5	D	553[A]	TP7	O4P-P-O1P	-2.29	100.55	109.39
6	D	552	F43	CAB-CBB-CCB	-2.27	108.72	113.59
6	D	552	F43	O8D-C7D-C6D	-2.19	117.28	120.86
12	C	1	PEG	C3-O2-C2	2.15	122.60	113.29
6	A	1	F43	C8C-C9C-CAC	-2.14	108.98	113.59
6	D	552	F43	C6D-C5D-C2D	-2.11	107.21	111.46
6	A	1	F43	C2D-C1D-CHD	2.09	124.52	121.85
6	A	1	F43	C9A-C2A-C3A	2.04	116.00	112.98
8	D	555[B]	SHT	OK-CK-N	2.03	125.04	122.35
5	A	553[A]	TP7	O1-C1-N	-2.02	119.55	122.95

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	555[B]	SHT	S1-CC-CD-SG2
8	A	555[B]	SHT	CK-CK1-CK2-CK3
8	D	555[B]	SHT	CK-CK1-CK2-CK3
6	A	1	F43	C3A-CAA-CBA-CCA
6	D	552	F43	C3A-CAA-CBA-CCA
10	B	445	EDO	O1-C1-C2-O2
10	F	251	EDO	O1-C1-C2-O2
10	D	556	EDO	O1-C1-C2-O2
10	F	1	EDO	O1-C1-C2-O2
8	A	555[B]	SHT	CK1-CK2-CK3-CK4
8	A	555[B]	SHT	CB-O3'-P-O8P
5	A	553[A]	TP7	CB-O4P-P-O3P
10	A	557	EDO	O1-C1-C2-O2
8	D	555[B]	SHT	S1-CC-CD-SG2
8	A	555[B]	SHT	CK5-CK6-SK-S1
8	D	555[B]	SHT	CK5-CK6-SK-S1

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Mol	Chain	Res	Type	Atoms
8	D	555[B]	SHT	CK1-CK2-CK3-CK4
5	D	553[A]	TP7	C2-C3-C4-C5
5	A	553[A]	TP7	C2-C3-C4-C5

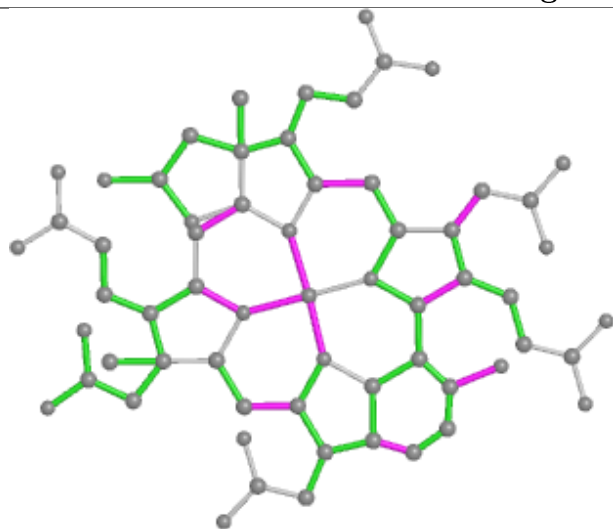
There are no ring outliers.

5 monomers are involved in 5 short contacts:

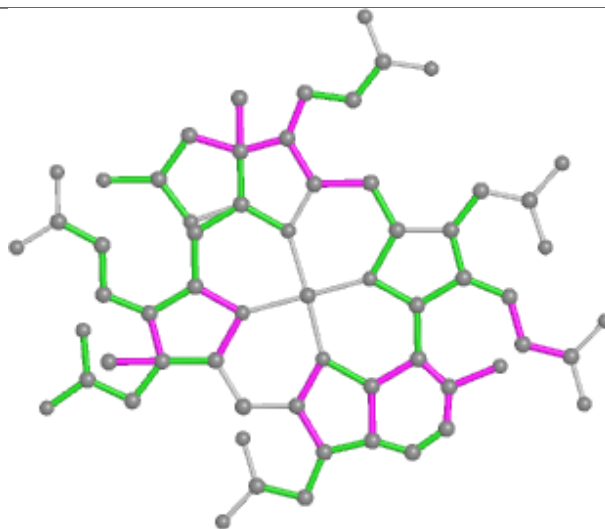
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	556	EDO	1	0
6	A	1	F43	2	0
8	D	555[B]	SHT	1	0
7	D	554[A]	COM	1	0
6	D	552	F43	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

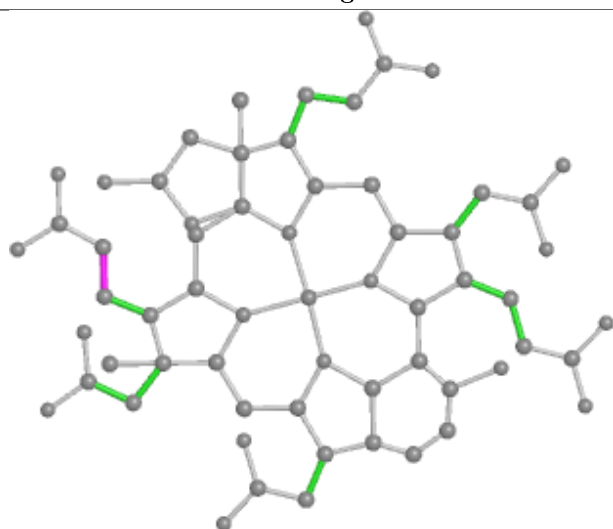
Ligand F43 A 1



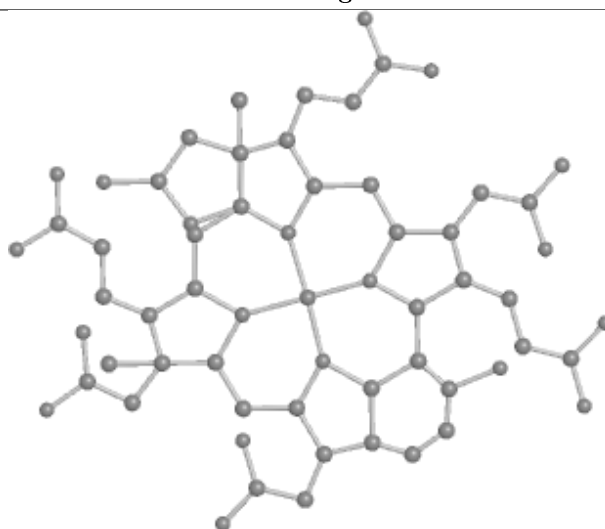
Bond lengths



Bond angles

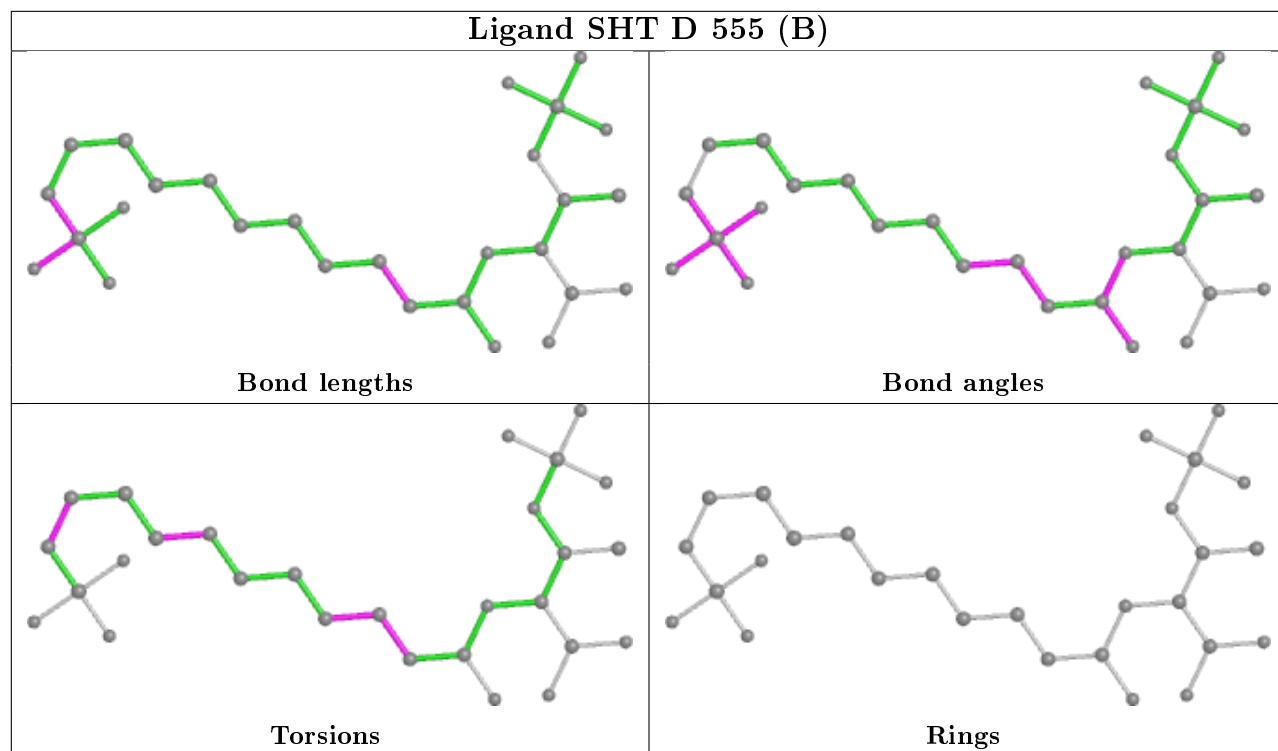


Torsions

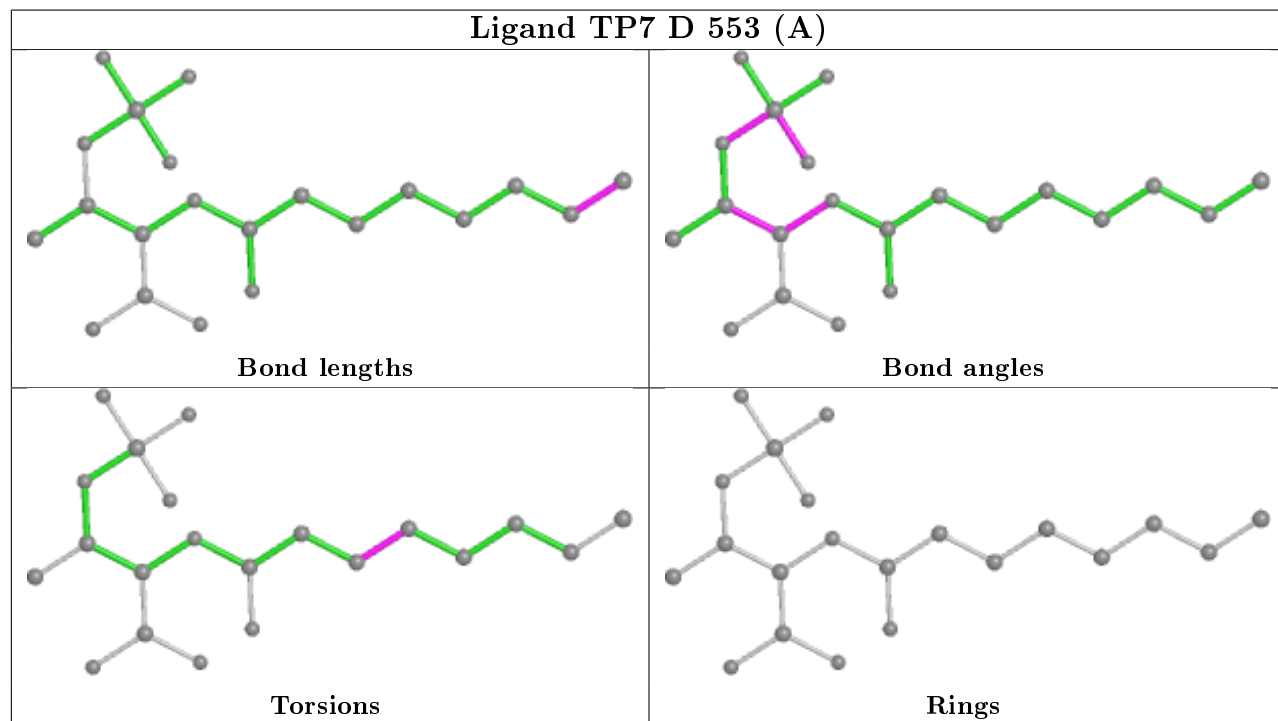


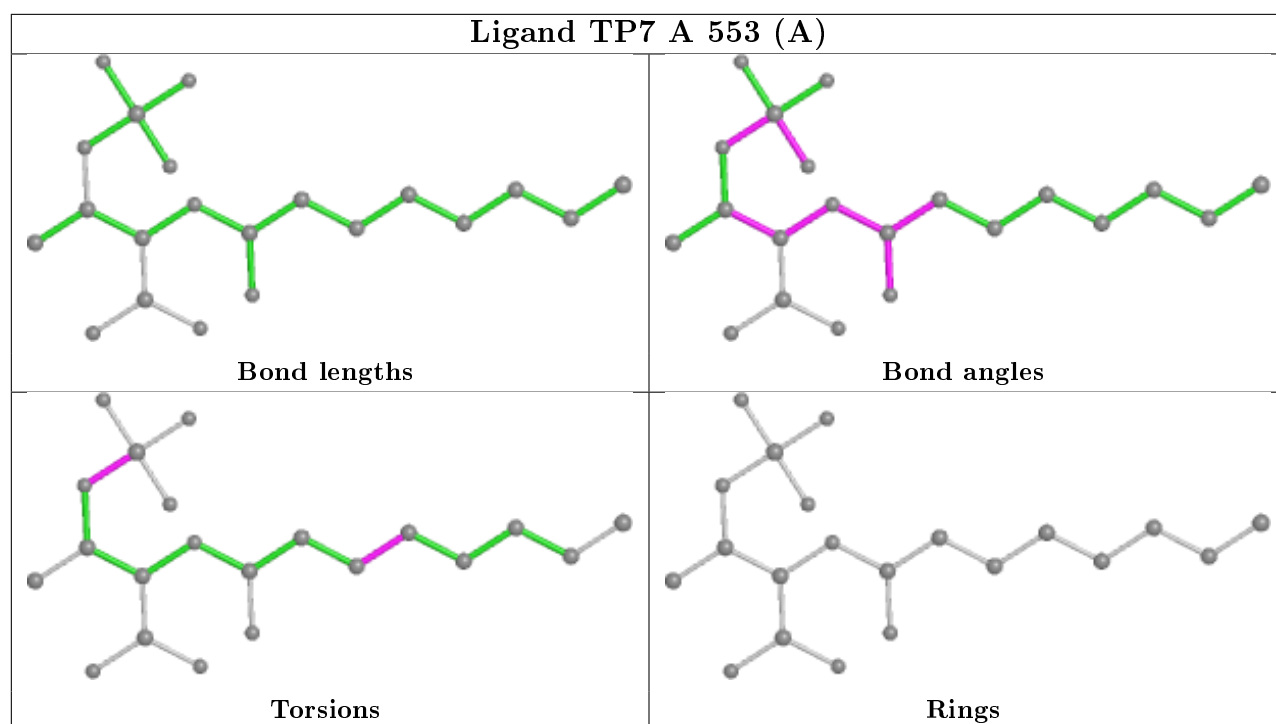
Rings

Ligand SHT D 555 (B)

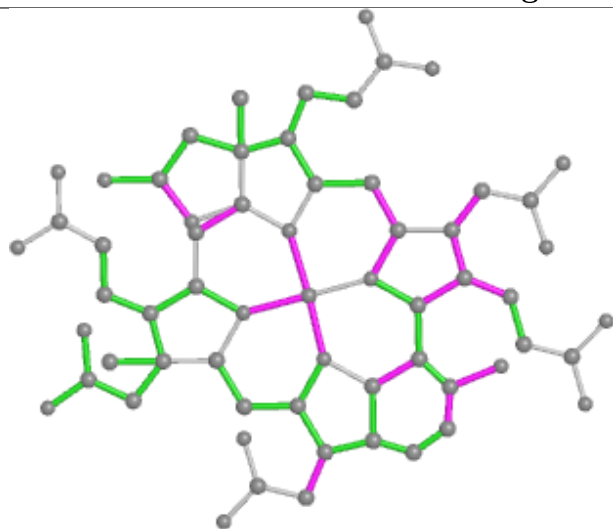


Ligand TP7 D 553 (A)

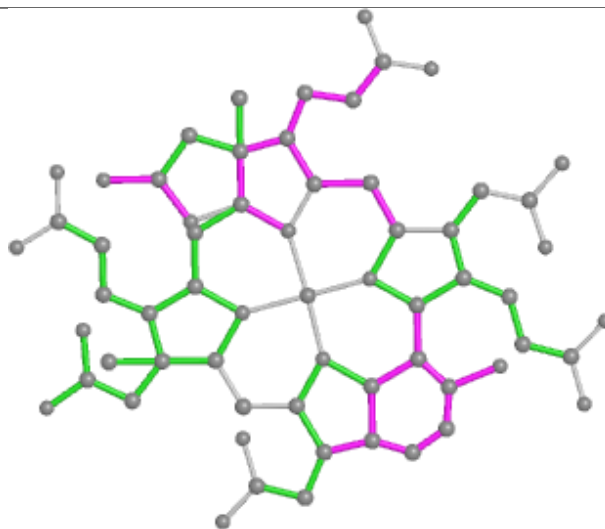




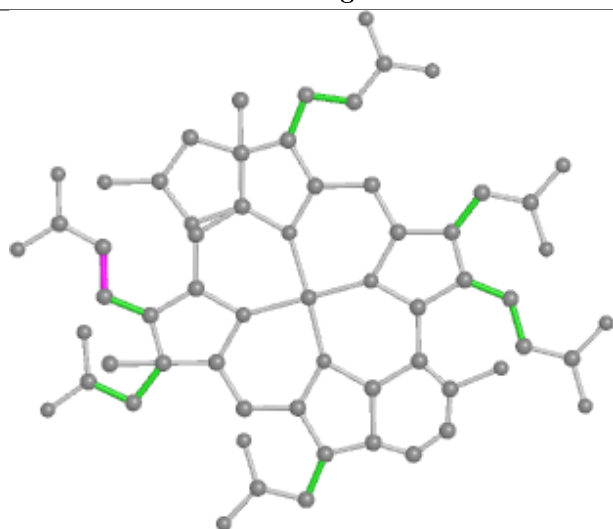
Ligand F43 D 552



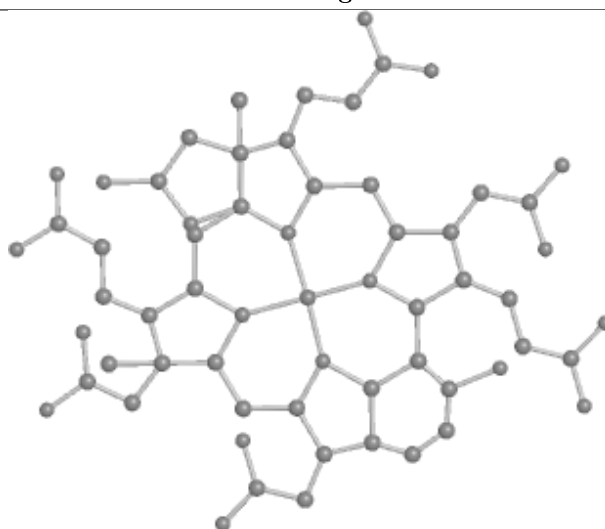
Bond lengths



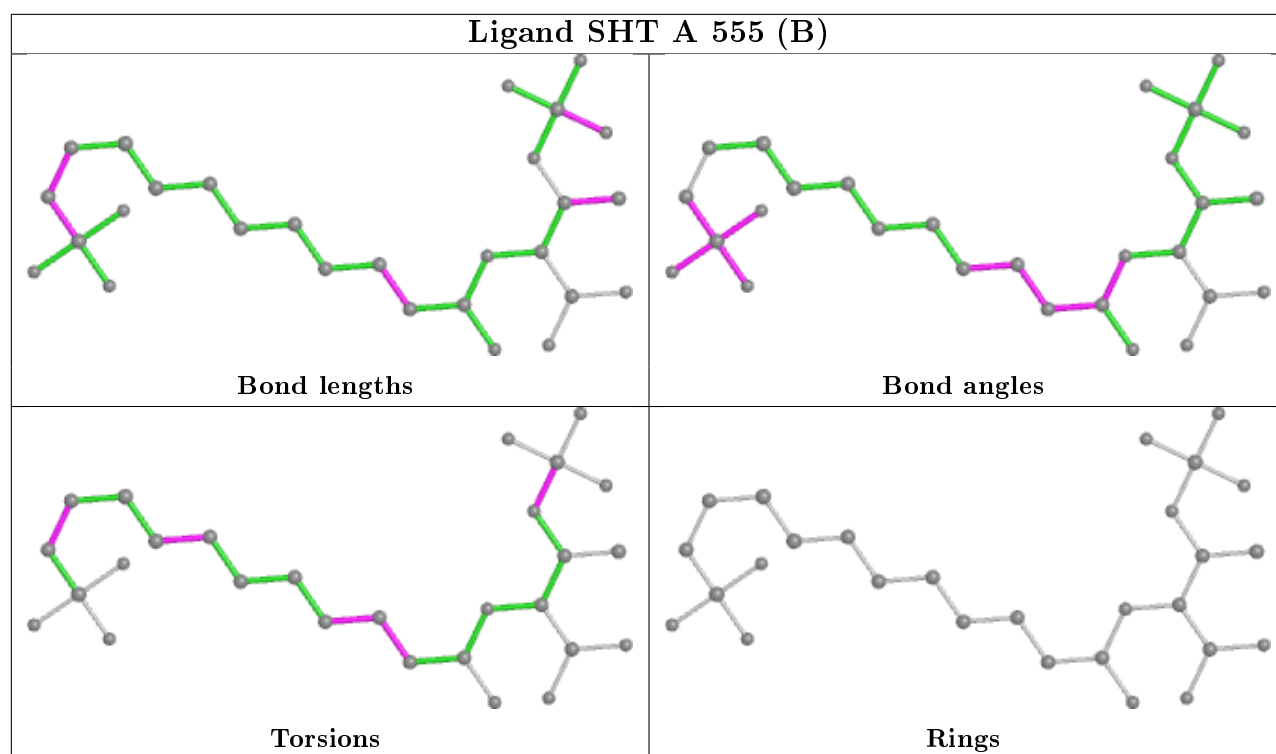
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/549 (98%)	-0.46	1 (0%) 95 95	6, 10, 21, 33	0
1	D	543/549 (98%)	-0.45	5 (0%) 84 87	6, 10, 20, 37	0
2	B	442/442 (100%)	-0.46	1 (0%) 95 95	7, 12, 21, 35	0
2	E	442/442 (100%)	-0.39	5 (1%) 80 84	7, 12, 23, 40	0
3	C	247/248 (99%)	-0.22	12 (4%) 29 33	9, 14, 32, 47	0
3	F	246/248 (99%)	-0.15	12 (4%) 29 33	8, 14, 30, 53	0
All	All	2463/2478 (99%)	-0.39	36 (1%) 73 78	6, 12, 23, 53	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	ASP	6.9
3	C	60	ASP	5.0
3	F	45	PRO	4.8
2	E	441	ASN	4.6
1	D	549	ALA	4.4
3	C	45	PRO	4.4
3	C	180	ASP	4.1
3	F	57	GLU	4.0
3	F	180[A]	ASP	3.6
2	B	98	ASP	3.4
3	C	62	PRO	3.3
2	E	2	ALA	3.2
1	A	2	ALA	3.0
3	F	63	GLU	2.9
3	C	208	GLU	2.8
3	C	46	GLY	2.8
2	E	97	GLU	2.7
3	C	63	GLU	2.7
3	F	46	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	297[A]	ASP	2.7
1	D	118	LYS	2.6
2	E	442	GLU	2.6
3	C	57	GLU	2.6
3	C	59	MET	2.5
1	D	2	ALA	2.5
3	F	62	PRO	2.4
3	C	179	LYS	2.4
3	F	196	ASP	2.3
3	C	248	LEU	2.3
1	D	24	THR	2.3
3	F	197	GLU	2.2
3	F	179[A]	LYS	2.2
1	D	15	GLU	2.1
3	F	207[A]	GLU	2.1
3	C	196	ASP	2.1
3	F	48	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MHS	A	257	11/12	0.97	0.05	8,10,14,17	0
1	AGM	D	271	12/13	0.97	0.07	6,7,7,8	0
1	MGN	D	400	10/11	0.98	0.05	6,8,8,8	0
1	MGN	A	400	10/11	0.98	0.05	7,8,9,10	0
1	MHS	D	257	11/12	0.98	0.05	9,10,12,16	0
1	AGM	A	271	12/13	0.98	0.05	6,6,7,8	0
1	SMC	A	452	7/8	0.99	0.05	7,7,9,10	0
1	GL3	A	445	4/5	0.99	0.06	6,7,7,8	0
1	SMC	D	452	7/8	0.99	0.05	7,8,9,11	0
1	GL3	D	445	4/5	0.99	0.06	6,6,7,7	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

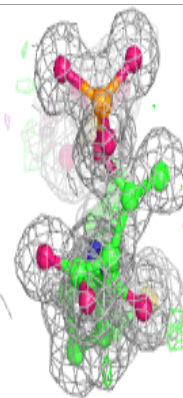
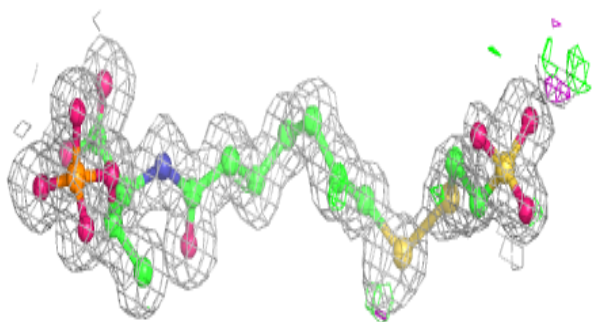
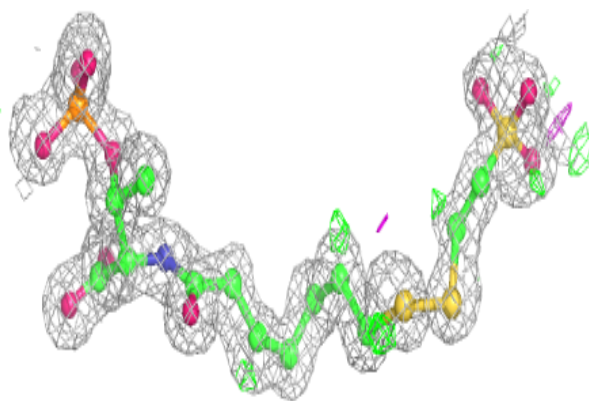
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	EDO	F	251	4/4	0.81	0.16	39,42,43,48	0
10	EDO	B	445	4/4	0.82	0.08	42,42,43,46	0
10	EDO	A	557	4/4	0.85	0.08	30,35,39,42	0
12	PEG	C	1	7/7	0.86	0.13	34,38,42,42	0
10	EDO	F	1	4/4	0.87	0.11	38,39,39,39	0
10	EDO	D	556	4/4	0.89	0.10	32,38,40,44	0
4	MG	B	444	1/1	0.97	0.15	23,23,23,23	0
4	MG	B	1[B]	1/1	0.97	0.19	21,21,21,21	1
4	MG	F	250	1/1	0.98	0.08	16,16,16,16	0
4	MG	E	444	1/1	0.98	0.20	22,22,22,22	0
8	SHT	A	555[B]	28/28	0.98	0.06	6,7,12,14	28
4	MG	C	250	1/1	0.98	0.10	17,17,17,17	0
4	MG	A	551[A]	1/1	0.98	0.22	18,18,18,18	1
9	ACT	A	556[B]	4/4	0.98	0.06	15,16,17,19	4
7	COM	D	554[A]	7/7	0.98	0.06	6,9,10,10	7
5	TP7	A	553[A]	21/21	0.98	0.06	5,7,7,8	21
4	MG	D	1	1/1	0.98	0.13	20,20,20,20	0
4	MG	A	552[B]	1/1	0.99	0.17	14,14,14,14	1
6	F43	A	1	62/62	0.99	0.05	6,8,11,13	0
6	F43	D	552	62/62	0.99	0.05	6,8,11,12	0
7	COM	A	554[A]	7/7	0.99	0.04	8,9,12,12	7
4	MG	D	551	1/1	0.99	0.17	18,18,18,18	0
8	SHT	D	555[B]	28/28	0.99	0.05	6,7,11,13	28
5	TP7	D	553[A]	21/21	0.99	0.05	4,6,8,8	21
11	ZN	A	558	1/1	1.00	0.03	10,10,10,10	1

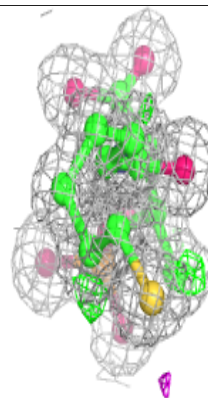
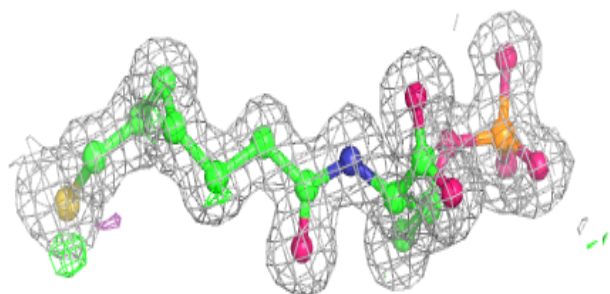
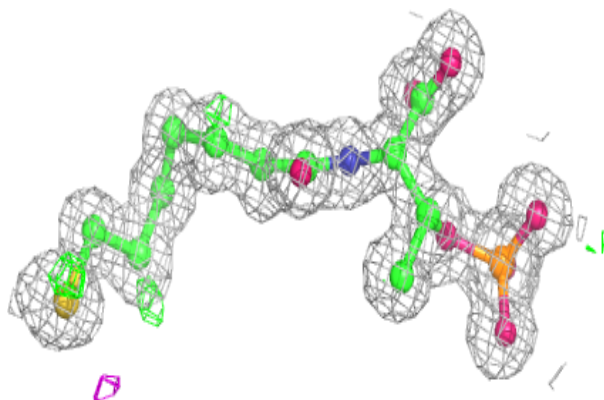
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SHT A 555 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

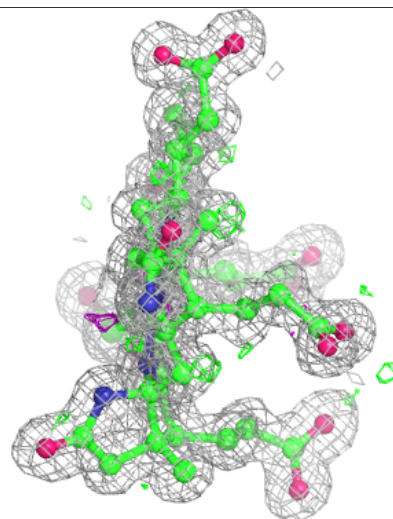
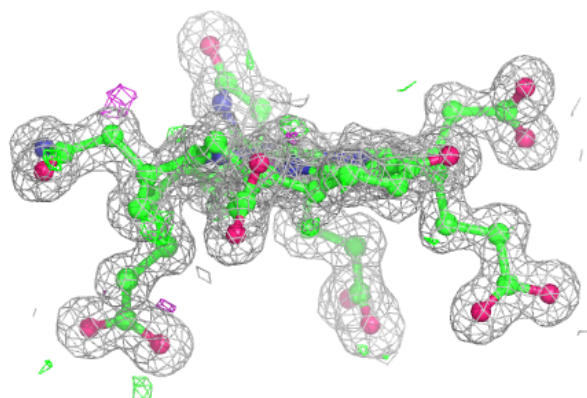
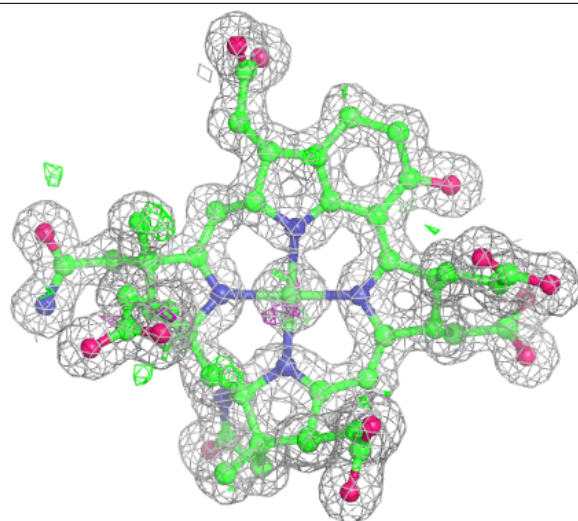
**Electron density around TP7 A 553 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



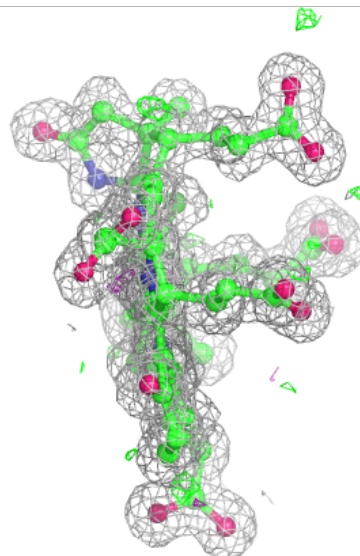
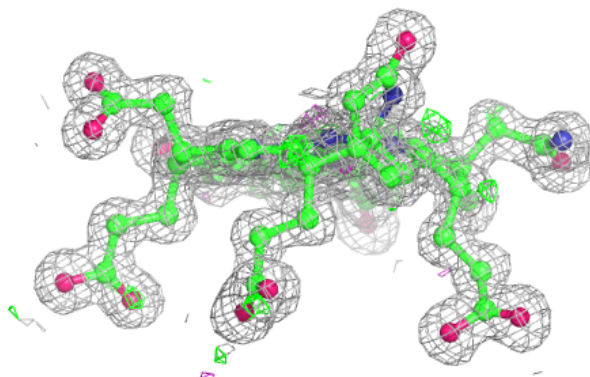
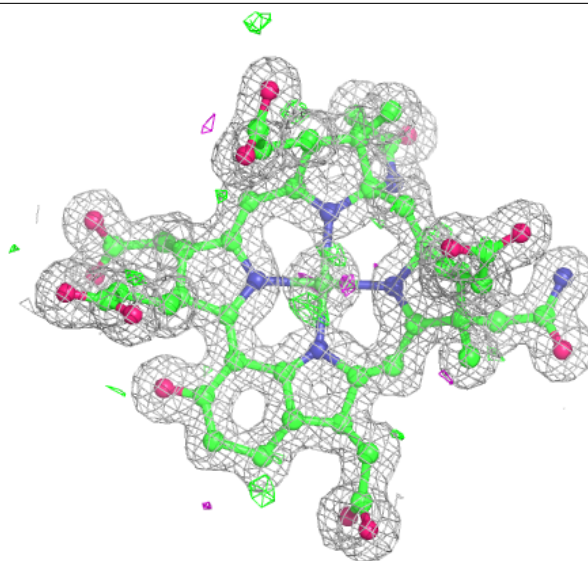
Electron density around F43 A 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



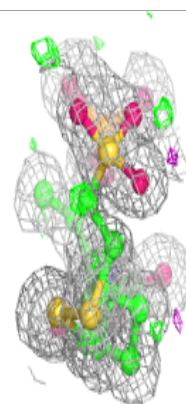
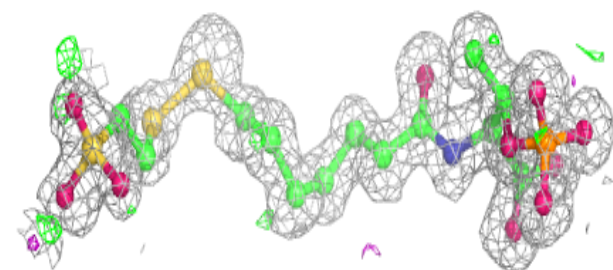
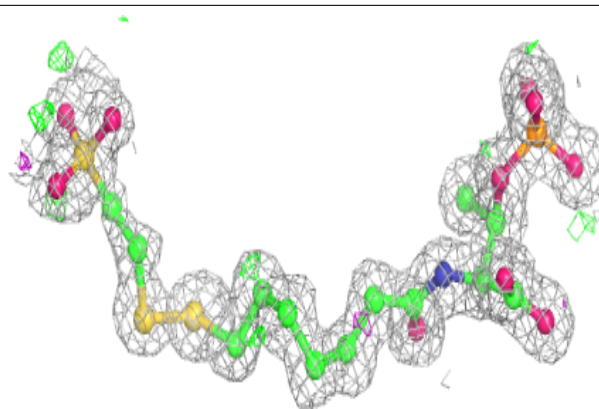
Electron density around F43 D 552:

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and green (positive)

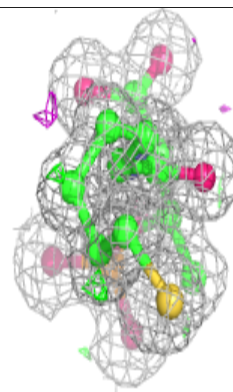
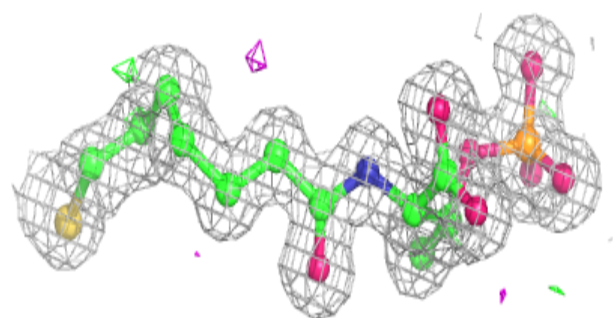
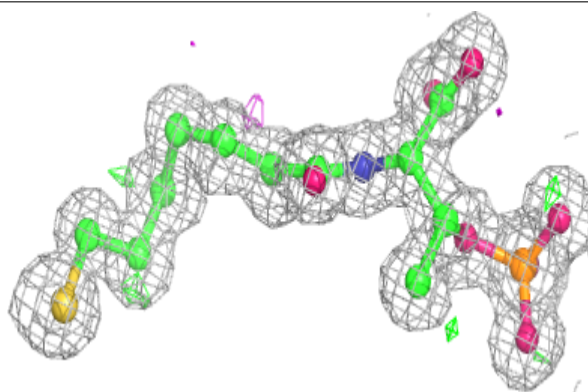


Electron density around SHT D 555 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TP7 D 553 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.